(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
9 February 2006 (09.02.2006)

PCT

(10) International Publication Number
WO 2006/015258 A2

(51) International Patent Classification:
C12N 9/00 (2006.01)

(21) International Application Number:
PCT/US2005/027084

(22) International Filing Date: 28 July 2005 (28.07.2005)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/592,297 28 July 2004 (28.07.2004) US
60/592,269 29 July 2004 (29.07.2004) US

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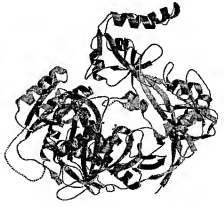
(81) Designated States *(unless otherwise indicated, for every kind of national protection available)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(84) Designated States *(unless otherwise indicated, for every kind of regional protection available)*: ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:
— *without international search report and to be republished upon receipt of that report*

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: METHODS AND COMPOSITIONS RELATED TO ARGONAUTE PROTEINS



(57) Abstract: This invention provides methods and compositions related to Argonaute proteins and, in certain embodiments, the applications of these methods and compositions to treatment and therapeutics based on RNAi.

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METHODS AND COMPOSITIONS RELATED TO ARGONAUTE PROTEINS

RELATED APPLICATIONS

This application claims the benefit of priority to U.S. Provisional Patent Application Nos. 60/592,269, filed on July 29, 2004, and 60/592,297, filed on July 28, 2004, which applications are hereby incorporated by reference in their entireties.

BACKGROUND OF THE APPLICATION

The presence of double-stranded RNA (dsRNA) in most eukaryotic cells provokes a sequence-specific silencing response known as RNA interference (RNAi) (G.J. Hannon, Nature 418, 244 (2002); A. Fire et al., Nature 391, 806 (1998)). The dsRNA trigger of this process can be derived from exogenous sources or transcribed from endogenous non-coding RNA genes that produce microRNAs (miRNAs) (Hannon, *supra*; G. Hutvagner et al., Curr. Opin. Genet. Dev. 12, 225 (2002)). RNAi begins with the conversion of dsRNA silencing triggers into small RNAs of ~21-26 nt in length (A. Hamilton et al., Embo J. 21, 4671 (2002)). This is accomplished by processing of triggers by specialized RNaseIII family nucleases, Dicer and Drosha (E. Bernstein et al., Nature 409, 363 (2001); Y. Lee et al., Nature 425, 415 (2003)). Resulting small RNAs join an effector complex, known as RISC (RNA-Induced Silencing Complex) (S.M. Hammond et al., Nature 404, 293 (2000)). Silencing by RISC can occur via several mechanisms. In flies, plants and fungi, dsRNAs can trigger chromatin remodeling and transcriptional gene silencing (M.F. Mette et al., Embo J. 19, 5194 (2000); I.M. Hall et al., Science 297, 2232 (2002); T. Volpe et al., Science 22, 22 (2002); M. Pal-Bhadra et al., Mol. Cell 9, 315 (2002)). RISC can also interfere with protein synthesis, and this is the predominant mechanism used by miRNAs in mammals (P.H. Olsen et al., Dev. Biol. 216, 671 (1999); D.P. Bartel, Cell 116, 281 (2004)). However, the best-studied mode of RISC action is mRNA cleavage (T. Tuschl et al., Genes Dev. 13, 3191 (1999); P.D. Zamore, Cell 101, 25 (2000)). When programmed with a small RNA that is fully

complementary to the substrate RNA, RISC cleaves that RNA at a discrete position, an activity that has been attributed to an unknown RISC component, "Slicer" (S.M. Elbashir et al., Embo J. 20, 6877 (2001); J. Martinez et al., Cell 110, 563 (2002)). Whether or not RISC cleaves a substrate can be determined by the degree of complementarity between the siRNA and mRNA, as mismatched duplexes are often not processed (Elbashir et al., *supra*). However, even for mammalian miRNAs, which normally repress at the level of protein synthesis, cleavage activity can be detected with a substrate that perfectly matches the miRNA sequence (G. Hutvagner et al., Science 1, 1 (2002)). This prompted the hypothesis that all RISCs are equal with the outcome of the RISC-substrate interaction being determined largely by the character of the interaction between the small RNA and its substrate.

RISC contains two signature components. The first is the small RNA, which co-fractionated with RISC activity in Drosophila S2 cell extracts (Hammond et al., *supra*) and whose presence correlated with dsRNA-programmed mRNA cleavage in Drosophila embryo lysates (Tuschl et al., *supra*; Zamore et al., *supra*). The second is an Argonaute protein, which was identified as a component of purified RISC in Drosophila (S.M. Hammond et al., Science 293, 1146 (2001)). Subsequent studies have suggested that Argonautes are also key components of RISC in mammals, fungi, worms, protozoans and plants (Martinez et al., *supra*; M.A. Carmell et al., Nat. Struct. Mol. Biol. 11, 214 (2004)). To date, the identity of "Slicer" and the function of Argonaute proteins are unknown.

BRIEF SUMMARY OF THE APPLICATION

This application provides methods and compositions related to Argonaute proteins.

A first aspect of application provides a crystalline Argonaute. Certain embodiments provide an isolated and purified Argonaute protein having a three-dimensional structure defined by the atomic coordinates such as for example as shown in Table 3. The crystalline Argonaute may comprise an archae Argonaute protein. Alternatively, the crystalline Argonaute may comprise a mammalian Argonaute protein, e.g., a human Argonaute protein such as human Ago-2.

Examples of mammalian Argonaute proteins may be Ago-1, Ago-2, Ago-3, or Ago-4.

In certain embodiments, a crystalline Argonaute may comprise an Argonaute protein having an amino acid sequence that is 95% identical to SEQ ID NO: 2 (or human Ago-2) or a homologue, fragment, variant, or derivative thereof. Alternatively, a crystalline Argonaute may comprise an Argonaute protein having an amino acid sequence that is 95% identical to SEQ ID NO: 2 (or human Ago-2) or a homologue, fragment, variant, or derivative thereof.

Certain embodiments provide a crystalline Argonaute comprising a three-dimensional structure defined by all or a portion of the atomic co-ordinates such as for example as set forth in Table 3.

The application also provides native crystals, derivative crystals or co-crystals, that have a root mean square deviation ("r.m.s.d.") of less than or equal to about 1.5 Angstrom when superimposed, using backbone atoms (N, Cα, C and O), on the structure coordinates listed in Table 3.

A crystalline Argonaute of the application may comprise at least two domains, e.g., a PAZ domain and a PIWI domain. A PIWI domain comprises a carboxylate triad formed by the motif "DDX" (X refers to a third amino acid, e.g., E). A crystalline Argonaute of the application may comprise a PIWI domain having a carboxylate triad formed by D597, D669, and a third amino acid.

A crystalline Argonaute of the application may comprise the following overall architecture: the N-terminus, middle, and PIWI domains form a crescent-shaped base; and the PAZ domain is positioned above the crescent shaped base; resulting in a cleft between said crescent-shaped base and the PAZ domain.

In certain embodiments, a crystalline Argonaute permits an X-ray crystallography resolution better than 2.25 Angstrom.

In certain embodiments, a crystalline Argonaute is soaked with one or more agents to form co-complex structures.

A crystalline Argonaute may comprise a PIWI domain having an active site defined by two or more amino acids, such as for example the "DDX" (X representing a third amino acid, e.g., E) triad. A crystalline Argonaute may comprise a PAZ domain having an active site defined by two or more amino acids. In certain embodiments, an active site is capable of accommodating an agent, e.g., a ligand or an inhibitor. A ligand or an inhibitor may be a nucleic acid molecule, a peptidomimetic, or a small organic molecule. A ligand or an inhibitor may be soaked in to form a co-complex. A nucleic acid molecule that is a ligand or an inhibitor can be a single stranded RNA molecule, e.g., a single stranded RNA molecule comprising between 15-50 nucleotides.

The application further provides an isolated complex comprising an Argonaute protein and a single stranded RNA molecule hybridized to its target nucleic acid. In certain embodiments, the single stranded RNA molecule is bound to the PAZ domain of the Argonaute protein. In certain embodiments, the target nucleic acid further interacts with the crescent-shaped base of the Argonaute protein.

A further aspect of the application provides a method of determining the three-dimensional structure of an Argonaute protein or a mutant, derivative, variant, analogue, homologue, sub-domain or fragment thereof. The method may comprise aligning the amino acid sequence of the Argonaute mutant, derivative, variant, analogue, homologue, sub-domain or fragment with the amino acid sequence of PfAgo or as set forth in SEQ ID NO: 5 to match homologous regions of the amino acid sequences. The method may further comprise modeling the structure of the matched homologous regions of said target Argonaute protein of unknown structure on the corresponding regions of the Argonaute protein structure as defined by the atomic co-ordinates as set forth in Table 3. The method may also comprise determining a conformation for the Argonaute mutant, derivative, variant, analogue, homologue, sub-domain or fragment which substantially preserves the structure of said matched homologous regions.

A further aspect of the application provides a method of identifying an agent that binds an Argonaute protein. The method may comprise applying a 3-dimensional molecular modeling algorithm to the atomic coordinates of an

Argonaute protein shown in Table 3 to determine the spatial coordinates of the binding pocket of the Argonaute protein. The method may further comprise electronically screening the stored spatial coordinates of a set of candidate agents against the spatial coordinates of the Argonaute protein binding pocket to identify agents that can bind to the Argonaute protein.

The application also provides a computer-based method for the analysis of the interaction of a molecular structure with an Argonaute protein. The method may comprise providing a structure comprising a three-dimensional representation of said Argonaute protein or a portion thereof, which representation comprises all or a portion of the coordinates set forth in Table 3. The method may further comprise providing a molecular structure to be fitted to said Argonaute protein structure. The method may also comprise fitting the molecular structure to the Argonaute protein structure, e.g., as set forth in the three-dimensional representation.

The application also provides a computer-readable storage medium encoded with the atomic coordinates or an Argonaute protein as shown in Table 3. Other embodiments also provide a data array comprising the atomic coordinates of an Argonaute protein as set forth in Table 3.

The application further provides an electronic representation of a crystal structure of an Argonaute protein. In certain embodiments, the electronic representation may contain atomic coordinate set forth in Table 3. Certain embodiments also provide an electronic representation of a binding site of the Argonaute protein. The binding site may locate in or be defined by the PAZ and/or PIWI domain or a portion thereof. Certain embodiments also provide an electronic representation of a domain of the Argonaute protein, e.g., a PIWI domain and/or a PAZ domain. Certain embodiments also provide an electronic representation of an agent in a binding site of an Argonaute protein, e.g., an active site of the Argonaute protein.

The crystal structure, the electronic representation, as well as other aspects of the application also relate to a method for identifying, designing, and/or optimizing

an RNAi construct or RNAi therapeutic of the invention, e.g., to improve an RNAi therapeutic's pharmacokinetic and/or pharmacodynamic profile.

Another aspect of the application relates to a method of obtaining a crystal formed by an Argonaute protein. The crystal may be grown using a precipitant. The crystal may be grown in a buffer, the pH of which buffer may be varied. The crystal may also be grown in the presence of a ligand or an inhibitor that interacts with the Argonaute protein, e.g., a domain of the Argonaute protein. The quality of the crystal can be improved by microseeding.

A further aspect of the application relates to a method of identifying an agent that modulates the activity of an RNAi construct. The method may comprise identifying an agent that modulates the expression and/or activity of an Argonaute protein. The method may involve an Argonaute protein expressed in a cell. The expressed Argonaute protein may be endogenous or exogenous to the cell. In certain embodiments, the agent can modulate (e.g., increase) the RNase activity of the Argonaute protein. The agent may alternatively or further modulate (e.g., increase) the expression of said Argonaute gene. In certain embodiments, an agent modulates the RNase activity and/or expression of an Argonaute protein in a tissue or cell type-specific manner.

In certain embodiments, the application relates to a method of identifying an agent that modulates the activity of an RNAi therapeutic. The method may comprise identifying an agent that modulates the expression and/or activity of an Argonaute protein. The method may involve an Argonaute protein expressed in a cell. The expressed Argonaute protein may be endogenous or exogenous to the cell. In certain embodiments, the agent can modulate (e.g., increase) the RNase activity of the Argonaute protein. The agent may alternatively or further modulate (e.g., increase) the expression of said Argonaute gene. In certain embodiments, an agent modulates the RNase activity and/or expression of an Argonaute protein in a tissue or cell type-specific manner.

In certain embodiments, an RNAi construct or an RNAi therapeutic attenuates the expression of a target nucleic acid molecule. The attenuation may be

by 2, 3, 5, 10, or higher fold. The target nucleic acid molecule may comprise an endogenous nucleic acid molecule. Alternatively, the target nucleic acid molecule is a heterologous to the genome of the cell. The heterologous nucleic acid molecule may be a nucleic acid from a pathogen.

An RNAi construct or an RNAi therapeutic of the application may comprise a nucleotide sequence at least 15 nucleotides in length that hybridizes to a target nucleic acid molecule. In certain embodiments, an RNAi construct or an RNAi therapeutic may comprise a hairpin nucleic acid. An RNAi construct or an RNAi therapeutic of the application may also comprise a promoter operably linked to a nucleotuide sequence that hybridizes to a target nucleic acid molecule. The promoter may be tissue or cell type-specific.

A further aspect of the application relates to a method of identifying an agent that potentiates the activity of an RNAi construct. The method may comprise identifying an agent that increases the expression and/or activity of an Argonaute protein. The agent may increase the expression and/or activity of an Argonaute protein in a tissue or cell type-specific manner.

Certain embodiments provides a method of identifying an agent that potentiates the activity of an RNAi therapeutic. The method may comprise identifying an agent that increases the expression and/or activity of an Argonaute protein. The agent may increase the expression and/or activity of an Argonaute protein in a tissue or cell type-specific manner.

Another aspect of the application provides a method of identifying an agent that modulates the activity of an RNAi construct. The method may comprise providing an isolated or recombinant Argonaute protein and assaying the RNase activity of the Argonaute protein in the presence of a candidate agent. A change in the RNase activity of the Argonaute protein in the presence of a candidate agent is indicative of the candidate agent capable of modulating the activity of the RNAi construct. The change may be relative to the RNase activity of the Argonaute protein in the absence of the candidate agent or a baseline or control level of the RNase activity of Argonaute protein. The method may involve an Argonaute

protein expressed in a cell. Alternatively, the method may involve an isolated or purified Argonaute protein. The method may further comprise determining the RNase activity of said Argonaute protein in the absence of a candidate agent. The identified agent may modulate the activity of an RNAi construct in a tissue or cell type-specific manner.

Certain embodiments provide a method of identifying an agent that modulates the activity of an RNAi therapeutic. The method may comprise providing an isolated or recombinant Argonaute protein and assaying the RNase activity of the Argonaute protein in the presence of a candidate agent. A change in the RNase activity of the Argonaute protein in the presence of a candidate agent is indicative of the candidate agent capable of modulating the activity of the RNAi therapeutic. The change may be relative to the RNase activity of the Argonaute protein in the absence of the candidate agent or a baseline or control level of the RNase activity of Argonaute protein. The method may involve an Argonaute protein expressed in a cell. Alternatively, the method may involve an isolated or purified Argonaute protein. The method may further comprise determining the RNase activity of said Argonaute protein in the absence of a candidate agent. The identified agent may modulate the activity of an RNAi construct in a tissue or cell type-specific manner.

A further aspect of the application provides a composition for targeted gene inhibition comprising an agent that modulates the RNase activity of an Argonaute protein. The composition may further comprise an RNAi construct or an RNAi therapeutic targeting a gene. In certain embodiments, an agent may potentiate the RNase activity of the Argonaute protein. Alternatively, an agent may inhibit the RNase activity of the Argonaute protein. In certain embodiments, the RNAi construct or therapeutic may target a gene in a first tissue or cell type; the identified agent may potentiate the RNase activity of the Argonaute protein in said first tissue or cell type. In certain embodiments, the identified agent may inhibit the RNase activity of the Argonaute protein in a second tissue or cell type.

The application also provides a pharmaceutical preparation comprising the compositions described herein and a physiologically acceptable carrier.

A further aspect of the invention relates to a cell line that overexpresses an Argonaute protein. The cell line of claim may overexpress a mammalian Argonaute protein, e.g., a human Agonaute protein. A mammalian Agonaute protein may be Ago-1, Ago-2, Ago-3, or Ago-4. The cell line may alternatively overexpress an Argonaute protein having an amino acid sequence that is 95% identical to an amino acid sequence as set forth in SEQ ID NOs.: 1-4, or a homologue, fragment, variant, or derivative thereof. The cell linc may alternatively overexpress an Argonaute protein encoded by a nucleic acid molecule having a sequence that is 95% identical to a nucleic acid sequence as set forth in any one of SEQ ID NOs.: 1-4. The cell line may alternatively overexpress an Argonaute protein encoded by a nucleic acid molecule that hybridizes under high stringency conditions to a nucleic acid sequence as set forth in any one of SEQ ID NOs.: 1-4. The cell line may alternatively overexpress an Argonaute protein having an amino acid sequence set forth in any one of SEQ ID NOs.: 1-4.

Another aspect of the application relates to a cell line that expresses a mutant Argonaute protein comprising an amino acid sequence that is different from a naturally-occurring Argonaute protein.

A further aspect of the application relates to a host (e.g., a cell or an animal) wherein the expression of an endogenous Argonaute protein is controlled by, e.g., a transgene (or a nucleic acid construct such as for example the construct based on the Puro PGK vector described herein).

The application also provides an assay for identifying nucleic acid sequences for conferring a particular phenotype in a cell, comprising constructing a library of nucleic acid sequences oriented to produce double stranded RNA. The assay may further comprise ntroducing a dsRNA library into a culture of target cells. The assay may also comprise identifying members of the library which confer a particular phenotype on the cell, and identifying the sequence from the cell which is identical or homologous to the library member.

Another aspect of the invention provides a nucleic acid composition comprising a first nucleic acid comprising an RNAi construct and a second nucleic

acid encoding an Argonaute protein. The RNAi construct may comprise a nucleotide sequence encoding a single-strand siRNA; the nucleotide sequence may be operably linked to a promoter. In certain embodiments, the second nucleic acid encodes a human Argonaute protein and may be operably linked to a promoter. Alternatively, the second nucleic acid may encode a non-naturally-occurring Argonaute protein. In certain embodiments, the RNAi construct may be tissue or cell type-specific. The promoters may be tissue or cell type-specific.

A further aspect of the application provides a cell expressing any of the nucleic acid compositions described herein.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1 shows the crystal structure of *Pyrococcus furiosus* Argonaute. Stereo ribbon representation of Argonaute with the N-terminal domain shown in blue, the "stalk" in light blue, the PAZ domain in red, the middle domain in green, the PIWI domain in purple and the interdomain connector in yellow. The active site residues are drawn in stick representation. Disordered loops are drawn as dotted lines. The N-terminal, middle and PIWI domains form a crescent base. The "stalk" holds the PAZ domain above the crescent base and the interdomain connector cradles the molecule. This figure as well as figures 2A, 3A,B, 5B were prepared with BobScript (60), MolScript (61) and Raster3D (62, 63).

Figs. 2A-2B show that the PAZ domains of PfAgo and hAgo1 have very similar structures. (Fig. 2A) Stereo diagram of the superposition of Ca atoms from the PAZ domain of PfAgo in shown in red and the PAZ domain of hAgo1 shown in gray. Dotted lines represent disordered regions. (Fig. 2B) Sequence alignment of the PAZ domains of PfAgo, hAgo1 and DmAgo2 based on the structural superposition of the three domains. The sequence of PfAgo-PAZ domain could not be readily aligned with PAZ domains from other species without knowledge of the structure. The secondary structure elements for PfAgo are shown above the sequence.

Figs. 3A-3C show that PIWI is an RNase H domain. (Fig. 3A) Ribbon diagrams of the PIWI domain, *E. coli* RNase HI and *M. jannaschii* RNase HII. The three

structures were superimposed and shown in a similar view with the secondary structure elements of the canonical RNase H fold in color. The active site residues are shown in stick representation. (Fig. 3B) A close-up view of the active sites. This view is rotated ~180° compared to the view in A. One active site aspartate is always located on β1 of the fold (the red strand) in this family of proteins and another aspartate is always located on β4 of the fold (the green strand). The third active site carboxylate, a glutamic acid, varies in its position. The Mg^{2+} ion in RNase HI is shown as a pink sphere. A strong difference electron density found in the active site of PIWI that was assigned as a water molecule is shown as a green sphere. (Fig. 3C) Sequence alignment of the PIWI domains from Pf Argonaute and the four human Argonaute proteins. Invariant residues are highlighted in purple and conserved residues are highlighted in blue. The secondary structure elements are shown above the structure. The conserved active site carboxylate residues are marked by a red asterisk.

Figs. 4A-4B show siRNA binding. (Fig. 4A) A 5'-phosphorylated ss-siRNA (4 nM) was radiolabled by phosphorylation with γ-^{32}P-ATP and hybridized with an unlabeled complementary strand to yield a ds-siRNA and was gel purified. The ss- and ds-siRNAs were UV-crosslinked to PfAgo and the adducts were resolved by SDS-PAGE. PfAgo binds preferentially to the ss-siRNA compared to the ds-siRNA. (Fig. 4B) Competition experiments were performed with the same labeled ss-siRNA and UV-crosslinking to PfAgo in the presence of increasing amounts of the indicated competitors (from 0 to 400 nM), showing preferential binding to a 5'-phosphorylated ss-siRNA compared to unphosphorylated ss-siRNA.

Figs. 5A-5C illustrate a model for siRNA-guided mRNA cleavage by Argonaute. (Fig. 5A) Two views of the electrostatic surface potential of PfAgo indicating a positively charged groove suitable for interaction with nucleic acids. The locations of the domains are labeled and the approximate location of the active site in PIWI is marked by a yellow asterisk. The view on the left is slightly tilted on the horizontal axis compared to the view in Figure 1. Two of the loops were removed for a better view of the groove. The binding groove runs horizontally across the protein bending upwards between the PAZ and N-terminal domains on the right and bending around

between the PAZ and middle domains on the left. The view on the right is from the proposed exit groove of the mRNA and looking into the active site area (rotated ~90° compared to the view on the left). The PIWI domain is behind the middle domain in this view. The coloring scheme depicts potentials < -10 k_BT in red and > 10 k_BT in blue, where k_B is the Boltzman constant and T is the absolute temperature. This figure was prepared with GRASP (64).

(Fig. 5B) A model for si-RNA and mRNA binding. Argonaute is shown as a ribbon representation in gray. A 3' portion of the siRNA, shown in purple, was placed by superposition of the PAZ domain of the hAgo1-PAZ domain-RNA complex on the PAZ domain of PfAgo. The two nucleotides at the 3'-end of the siRNA are inserted in the PAZ cleft and the nucleotides 5' to those bind along the PAZ domain. The passenger strand of the hAgo1-PAZ complex placed in a similar manner was used to model the mRNA strand, shown in light blue, by extending the RNA 2 nucleotides at the 5'-end, and from the middle of that strand along the binding groove towards the active site in PIWI. The 5'- end of the mRNA is nested between the PAZ and N-terminal domains, across the stalk. The phosphate between the 11th and 12th nucleotides from the 5'-end of the mRNA falls near the active site residues shown in red.

(Fig. 5C) Schematic depiction of the model for siRNA-guided mRNA cleavage. The domains are colored as in Fig. 1. The siRNA, shown in yellow, binds with its 3'-end in the PAZ cleft and the 5' is predicted to reach the other end of the molecule and likely bind there. The mRNA is depicted in brown, comes in between the N-terminal and PAZ domains and out between the PAZ and middle domain. The active site in the PIWI domain, depicted as scissors, cleaves the mRNA opposite the middle of the siRNA guide.

Fig. 6 shows sequence alignment of the PAZ domains of PfAgo, hAgo1 and DmAgo2 based on the structural superposition of the three domains. The sequence of PfAgo-PAZ domain could not be readily aligned with PAZ domains from other species without knowledge of the structure. Invariant residues are highlighted in purple and conserved residues are highlighted in blue. The secondary structure elements for PfAgo are shown above the sequence.

Fig. 7 shows sequence alignment of the PIWI domains from Pf Argonaute and the four human Argonaute proteins. Invariant residues are highlighted in purple and conserved residues are highlighted in blue. The secondary structure elements are shown above the structure. The conserved active site carboxylate residues are marked by a red asterisk. Accession numbers are as follows: PfAgo (AAL80661), hAgo1 (NM_012199), hAgo2 (NM_012154), hAgo3 (NM_024852) and hAgo4 (NM_017629).

Fig. 8 shows another view of the electrostatic surface potential of PfAgo shown from the proposed exit groove of the mRNA and looking into the active site area (rotated ~90° around y and ~20° around x compared to the in Fig. 4A). The PIWI domain is behind the middle domain in this view.

Fig. 9 shows that only mammalian Ago2 can form cleavage-competent RISC. Panel A: The miRNA populations associated with Ago1, Ago2 and Ago3 were measured by microarray analysis as described in Methods. The heat map shows normalized log-ratio values for each dataset, with yellow representing increased relative amounts, and blue indicating decreased amounts, relative to the median. The top 25 log-ratios are shown in the expanded region. In each panel, "control" indicates parallel analysis of cells transfected with a vector control. Panel B: 293T cells were transfected with a control vector or with vectors encoding myc-tagged Ago1, Ago2 or Ago3, as indicated, along with an siRNA that targets firefly luciferase. Immunoprecipitates were tested for siRNA directed mRNA cleavage as described in Methods. Positions of 5' and 3' cleavage products are shown. Panel C: Immunoprecipitates as in Panel B were tested for in vivo siRNA binding by Northern blotting of Ago immunoprecipitates (see Methods). Panel D: Western blots of transfected cell lysates show similar levels of expression for each recombinant Argonaute protein.

Fig. 10 shows that Argonaute2 is essential for mouse development. Panel A: Total RNA from Wild-type or mutant embryos was tested for expression of Ago1, Ago2 or Ago3 by RT-PCR. Actin was also examined as a control. Panel B: At day E10.5, Ago2 null embryos show severe developmental delay as compared to heterozygous and wild-type littermates. These embryos also show a variety of developmental

defects including swelling inside the pericardial membrane (Panel C, h=heart, indicated by the arrow) and failure to close the neural tube (Panel D, Panel E). Arrows in Panel D indicate the edges of the neural tube that has failed to close. In caudal regions where the neural tube does close, it has an abnormal appearance, being wavy as compared to wild-type embryos (Panel E, compare wt and Ago2 -/-). Ago2 is expressed in most tissues of the developing embyo as measured by in situ hybridization (Panel F) or analysis of an Ago2 gene trap animal (Panel G). In Panel F, f=forebrain, b=branchial arches, h=heart and lb=limb bud, all of which are relative hot spots for Ago2 mRNA. In Panel G, the left embryo shows similar patterns when staining for the gene-trap marker, β-galactosidase, proceeds for only a short period. Longer incubation (Panel G, right) gives uniform staining throughout the embryo.

Fig. 11 shows that Argonaute2 is essential for RNAi in MEF. Panel A: RT-PCR of mRNA prepared from Wild-type or Ago2-/- MEF reveals consistent expression of Ago1 and Ago3 but a specific lack of Ago2 expression in the null MEF. Actin mRNA serves as a control. Panel B: Wild-type and mutant MEFs were co-transfected with plasmids encoding Renilla and firefly luciferases either with or without firefly siRNA as indicated. Ratios of firefly to Renilla activity, normalized to 1 for the no-siRNA control were plotted. For each genotype, the ability of Ago1 and Ago2 to rescue suppression was tested by co-transfection with expression vectors encoding each protein as indicated. Panel C: NIH-3T3 cells, Wild-type MEF or Ago2 mutant MEF were tested as described in B (except that Renilla/firefly ratios are plotted) for their ability to suppress a reporter of repression at the level of protein synthesis. In this case, the Renilla luciferase mRNA contains multiple, imperfect binding sites for a CXCR4 siRNA. Cells were transfected with a mixture of firefly and Renilla luciferase plasmids with or without (as indicated) the siRNA.

Fig. 12 shows mapping of the requirements for assembly of cleavage-competent RISC. Ago1, Ago2 or the indicated mutants of Ago2 were expressed as myc-tagged fusion proteins in 293T cells. In all cases, expression constructs were co-transfected with a luciferase siRNA. Western Blotting (not shown) indicated similar expression for each mutant. Immunoprecipitate containing individual proteins were tested for

cleavage activity against a luciferase mRNA. Positions of 5' and 3' cleavage products are indicated. SiRNA binding was examined for each mutant by Northern blotting of immunoprecipitates or by staining of immunoprecipitates with Sybr Gold (Molecular Probes). Representatives for these assays are shown. In no case was a defect in interaction of mutants with siRNAs detected.

Fig. 13 shows that Argonaute2 is a candidate for Slicer. Panel A: Ago2 protein was immunoaffinity purified from transiently transfected 293T cells. The preparation contained two major proteins (Protein Gel), in addition to heavy and light chains. These were identified by mass spectrometry as Ago2 and HSP90. Immunoprecipitates were mixed (see Methods) in vitro with single- or double-stranded siRNAs or with a 21 nt DNA having the same sequence as the siRNA, as indicated. Reconstituted RISC was tested for cleavage activity with a uniformly labeled synthetic mRNA. Positions of 5' and 3' cleavage products are noted. Where indicated, the siRNA was not 5' phosphorylated and in one case, ATP was not added to the reconstitution reaction. Panel B: Ago2 or Ago2 mutants (as indicated) were assembled into RISC in vivo by co-transfection with siRNAs followed by immunoaffinity purification or by in vitro reconstitution, mixing affinity purified proteins with ss-siRNAs. These were tested for activity against a complementary mRNA substrate. 5' and 3' cleavage products are as in Panel A. Both mutant proteins were expressed at levels similar to wild-type Ago2 and bound siRNAs as readily (Panel C, Panel D) Ago2 (H634P) and (Q633R) behave similarly in this assay.

Fig. 14 shows cleavage by Ago2-containing RISC irrespective of siRNA sequence. Ago2-containing RISCs were formed in vivo by co-transfection. Complexes were recovered by immunoprecipitation and tested for cleavage activity with a uniformly labeled, synthetic mRNA. Positions of 5', and 3' cleavage products expected for each reaction are indicated.

Fig. 15 shows construction of Ago2 mutant mice. The insertional disruption strategy for inactivating mouse Ago2 is shown, along with a southern blot of DNA from wild-type, heterozygous, and null embryos. Probe is indicated by asterisk. For reference, PAZ domain is encoded by exons 5-8. The insertion duplicates exons 3-

6, which includes two exons of the PAZ domain, and inserts ~10 Kb of vector sequences into the gene, creating a high probability that any truncated protein that might be generated from this allele would be non-functional. Additionally, no Ago2 mRNA was detected from these cells by RT-PCR. However, all of the coding capacity of Ago2 does still exist in the mutant genome. Therefore, although all available evidence indicates a null mutation, the possibility cannot be completely ruled out that this mutant can still synthesize a small amount of Ago2, making it a severe hypomorph rather than a null. Southern blots showing the patterns for Wild-type, heterozygous and mutant animals are shown below the disruption strategy.

Fig. 16 shows expression analysis of Ago3 in embryos. Embryonic day 9.5 embryos were collected from timed matings of Wild-type animals. These were stained for expression of Ago3 mRNA by in situ hybridization as described in Methods. Ago3 shows the same expression pattern as is seen in parallel analyses of Ago2 mRNA expression (see Fig. 10, Panel F).

Fig. 17 shows that Ago2-mutant MEF are defective for siRNA-mediated repression WT and Ago2-mutant MEF (genotypes indicated on the left) were transfected with a combination of plasmids encoding dsRed and GFP, either with or without GFP siRNAs (as indictated on the right). Microscopic examination revealed consistent co-expression of dsRed and GFP in the absence of siRNAs in both WT and mutant cells. SiRNAs eliminated co-expression of GFP in WT cells but did not alter GFP expression in Ago2-/- cells.

Fig. 18 shows that intact Ago2 is required for formation of cleavage-competent RISC. Deletions within Ago2 are indicated schematically. Plasmids encoding epitope-tagged versions of each deletion mutant were co-transfected into 293T cells with an siRNA to firefly luciferase. Wild-type Ago2 was similarly expressed as a control. RISCs were immunoaffinity purified and tested for activity against a uniformly labeled mRNA substrate. Each protein was expressed as indicated by Western blotting with a myc antiserum, but none of the deletion mutants bound siRNAs, as determined by Nothern blotting of immunoprecipitates.

Fig. 19 shows that Ago2 can be reconstituted with different siRNAs. Ago2 was immunoaffinitity purified (see Fig. 13) and reconstituted in vitro with single stranded siRNAs that target either the sense strand or the antisense strand of a firefly luciferase mRNA. Similar complexes were formed in parallel with purified Ago1. In each case, Ago2 cleaved the complementary mRNA, whereas Ago1 complexes were inert. Positions of 5', and 3' cleavage products are indicated.

Fig. 20 shows that RISC is a metal-dependent nuclease. As previously shown, RISC requires a divalent metal for activity (Hannon, *supra*). Similarly, RISC, reconstituted in vitro with single-stranded siRNAs, depends on Mg++ for activity, as indicated by the ability to inhibit the complex with EDTA but not with EGTA (as indicated).

Fig. 21 shows that active site residues are conserved among Ago proteins. Putative active site aspartate residues in the PIWI domain were identified with reference to the structure of the *P. furiosus* Ago protein. These were also conserved in Ago proteins from a variety of species. Additionally, residues identified by a mutational analysis (e. g. H634) were also highly conserved.

Fig. 22 shows sequence alignment of mammalian Ago1 family members. An alignment of the protein sequences of human Argonautes1-4 highlights a very high degree of sequence conservation. Red indicates highly conserved, blue moderately conserved residues. Residues mutated in Ago2 in this study are indicated in green and by asterisks (see below). The PAZ domain is indicated by the yellow bar and the PIWI by the orange bar (boundaries set as determined by structural data). Accession numbers for individual genes are as follows: Ago1 (NM_012199), Ago2 (NM_012154), Ago3(NM_024852), Ago4 (NM_017629).

Fig. 23 shows Table 1 which provides crystallographic statistics for Argonaute.

Fig. 24 shows Table 2 which provides additional crystallographic statistics for Argonaute.

Fig. 25 shows Table 3 which provides the atomic coordinates for Argonaute.

DETAILED DESCRIPTION OF THE APPLICATION

Overview

Argonautes are often present as multiprotein families and are identified by two characteristic domains, PAZ and PIWI (21). These proteins mainly segregate into two sub-families, comprising those that are more similar to either Arabidopsis Argonaute1 or Drosophila Piwi. The Argonaute family was first linked to RNAi through genetic studies in C. elegans, which identified Rde-1 as a gene essential for silencing (22). Subsequent placement of a Drosophila Argonaute protein in RISC (19) makes it desirable to explore the unknown roles of this protein family. Toward this end, this application provides methods and compositions related to Argonaute. These methods and compositions are based on results obtained from structural studies of Argonaute proteins, as well as biochemical, and genetic studies of a subfamily of Argonaute proteins in mammals. As used herein, the term "Argonaut" refers to a protein which (a) mediates an RNAi response and (b) has an amino acid sequence at least 50 percent identical, and more preferably at least 75, 85, 90 or 95 percent identical to SEQ ID NOs: 1-5.

Structural Studies of Argonaute

The crystal structure of Argonaute is useful for in silico screening of agents that bind to Argonaute and/or modulates its activity. The candidate agents generated from the in silico screening can be further screened in biochemical assays to select for agents that modulate the activity of Argonaute.

I. Crystallization and Structure Determination

X-ray crystallography is a method of solving the three dimensional structures of molecules. The structure of a molecule is calculated from X-ray diffraction patterns using a crystal as a diffraction grating. Three dimensional structures of protein molecules arise from crystals grown from a concentrated aqueous solution of that protein. The process of X-ray crystallography can include the following steps:

(a) synthesizing and isolating (or otherwise obtaining) a polypeptide;

(b) growing a crystal from an aqueous solution comprising the polypeptide with or without a modulator; and

(c) collecting X-ray diffraction patterns from the crystals, determining unit cell dimensions and symmetry, determining electron density, fitting the amino acid sequence of the polypeptide to the electron density, and refining the structure.

a. Production of Polypeptides

The Argonaute polypeptides described herein may be chemically synthesized in whole or part using techniques that are well-known in the art (see, e.g., Creighton (1983) Biopolymers 22(1):49-58).

Alternatively, methods which are well known to those skilled in the art can be used to construct expression vectors containing the native or mutated Argonaute polypeptide coding sequence and appropriate transcriptional/translational control signals. These methods include in vitro recombinant DNA techniques, synthetic techniques and in vivo recombination/genetic recombination. See, for example, the techniques described in Maniatis, T (1989). Molecular cloning: A laboratory Manual. Cold Spring Harbor Laboratory, New York. Cold Spring Harbor Laboratory Press; and Ausubel, F. M. et al. (1994) Current Protocols in Molecular Biology (John Wiley & Sons, Secaucus, N.J.).

A variety of host-expression vector systems may be utilized to express the Argonaute coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing the Argonaute domain coding sequence; yeast transformed with recombinant yeast expression vectors containing the Argonaute domain coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g., baculovirus) containing the Argonaute domain coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosaic virus, TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti

plasmid) containing the Argonaute domain coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities.

Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters, may be used in the expression vector. For example, when cloning in bacterial systems, inducible promoters such as pL of bacteriophage .lambda., plac, ptrp, ptac (ptrp-lac hybrid promoter) and the like may be used; when cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter may be used; when cloning in plant cell systems, promoters derived from the genome of plant cells (e.g., heat shock promoters; the promoter for the small subunit of RUBISCO; the promoter for the chlorophyll alb binding protein) or from plant viruses (e.g., the .sup.35S RNA promoter of CaMV; the coat protein promoter of TMV) may be used; when cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) may be used; when generating cell lines that contain multiple copies of the Argonaute domain DNA, SV40-, BPV- and EBV-based vectors may be used with an appropriate selectable marker.

Exemplary methods describing methods of DNA manipulation, vectors, various types of cells used, methods of incorporating the vectors into the cells, expression techniques, protein purification and isolation methods, and protein concentration methods are disclosed in detail in PCT publication WO 96/18738. This publication is incorporated herein by reference in its entirety, including any drawings. Those skilled in the art will appreciate that such descriptions are applicable to the present invention and can be easily adapted to it.

b. Crystal Growth

Crystals are grown from an aqueous solution containing the purified and concentrated Argonaute polypeptide by a variety of techniques. These techniques include batch, liquid, bridge, dialysis, vapor diffusion, and hanging drop methods. McPherson (1982) John Wiley, New York; McPherson (1990) Eur. J. Biochem.

189:1-23; Webber (1991) Adv. Protein Chem. 41:1-36, incorporated by reference herein in their entireties, including all figures, tables, and drawings.

The native crystals of the application are, in general, grown by adding precipitants to the concentrated solution of the polypeptide. The precipitants are added at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

For crystals of the application, exemplary crystallization conditions are described in the Examples. Those of ordinary skill in the art will recognize that the exemplary crystallization conditions can be varied. Such variations may be used alone or in combination. In addition, other crystallizations may be found, e.g., by using crystallization screening plates to identify such other conditions.

c. X-Ray Diffraction

The diffraction data from X-ray crystallography is generally obtained as follows. When a crystal is placed in an X-ray beam, the incident X-rays interact with the electron cloud of the molecules that make up the crystal, resulting in X-ray scatter. The combination of X-ray scatter with the lattice of the crystal gives rise to nonuniformity of the scatter; areas of high intensity are called diffracted X-rays. The angle at which diffracted beams emerge from the crystal can be computed by treating diffraction as if it were reflection from sets of equivalent, parallel planes of atoms in a crystal (Bragg's Law). The most obvious sets of planes in a crystal lattice are those that are parallel to the faces of the unit cell. These and other sets of planes can be drawn through the lattice points. Each set of planes is identified by three indices, hk1. The h index gives the number of parts into which the a edge of the unit cell is cut, the k index gives the number of parts into which the b edge of the unit cell is cut, and the 1 index gives the number of parts into which the c edge of the unit cell is cut by the set of hk1 planes. Thus, for example, the 235 planes cut the a edge of each unit cell into halves, the b edge of each unit cell into thirds, and the c edge of each unit cell into fifths. Planes that are parallel to the bc face of the unit cell are the 100 planes; planes that are parallel to the ac face of the unit cell are the

010 planes; and planes that are parallel to the ab face of the unit cell are the 001 planes.

When a detector is placed in the path of the diffracted X-rays, in effect cutting into the sphere of diffraction, a series of spots, or reflections, are recorded to produce a "still" diffraction pattern. Each reflection is the result of X-rays reflecting off one set of parallel planes, and is characterized by an intensity, which is related to the distribution of molecules in the unit cell, and hkl indices, which correspond to the parallel planes from which the beam producing that spot was reflected. If the crystal is rotated about an axis perpendicular to the X-ray beam, a large number of reflections is recorded on the detector, resulting in a diffraction pattern.

The unit cell dimensions and space group of a crystal can be determined from its diffraction pattern. First, the spacing of reflections is inversely proportional to the lengths of the edges of the unit cell. Therefore, if a diffraction pattern is recorded when the X-ray beam is perpendicular to a face of the unit cell, two of the unit cell dimensions may be deduced from the spacing of the reflections in the x and y directions of the detector, the crystal-to-detector distance, and the wavelength of the X-rays. Those of skill in the art will appreciate that, in order to obtain all three unit cell dimensions, the crystal must be rotated such that the X-ray beam is perpendicular to another face of the unit cell. Second, the angles of a unit cell can be determined by the angles between lines of spots on the diffraction pattern. Third, the absence of certain reflections and the repetitive nature of the diffraction pattern, which may be evident by visual inspection, indicate the internal symmetry, or space group, of the crystal. Therefore, a crystal may be characterized by its unit cell and space group, as well as by its diffraction pattern.

Once the dimensions of the unit cell are determined, the likely number of polypeptides in the asymmetric unit can be deduced from the size of the polypeptide, the density of the average protein, and the typical solvent content of a protein crystal, which is usually in the range of 30-70% of the unit cell volume.

The diffraction pattern is related to the three-dimensional shape of the molecule by a Fourier transform. The process of determining the solution is in

essence a re-focusing of the diffracted X-rays to produce a three-dimensional image of the molecule in the crystal. Since re-focusing of X-rays cannot be done with a lens at this time, it is done via mathematical operations.

The sphere of diffraction has symmetry that depends on the internal symmetry of the crystal, which means that certain orientations of the crystal will produce the same set of reflections. Thus, a crystal with high symmetry has a more repetitive diffraction pattern, and there are fewer unique reflections that need to be recorded in order to have a complete representation of the diffraction. The goal of data collection, a dataset, is a set of consistently measured, indexed intensities for as many reflections as possible. A complete dataset is collected if at least 80%, preferably at least 90%, most preferably at least 95% of unique reflections are recorded. In one embodiment, a complete dataset is collected using one crystal. In another embodiment, a complete dataset is collected using more than one crystal of the same type.

Sources of X-rays include, but are not limited to, a rotating anode X-ray generator such as a Rigaku RU-200 or a beamline at a synchrotron light source, such as the Advanced Photon Source at Argonne National Laboratory. Suitable detectors for recording diffraction patterns include, but are not limited to, X-ray sensitive film, multiwire area detectors, image plates coated with phosphorus, and CCD cameras. Typically, the detector and the X-ray beam remain stationary, so that, in order to record diffraction from different parts of the crystal's sphere of diffraction, the crystal itself is moved via an automated system of moveable circles called a goniostat. The three dimensional (x, y, z) coordinates of Argonaute are shown in Table 3 (Figure 25) in the standard Protein Data Bank (PDB) format. (Bernstain F. C., et al. J. Mol. Biol., 1977, 122, 535).

TABLE 3 –Atomic Coordinates (Figure 25).

Once a dataset such as the one in Table 3 (Figure 25) is collected, the information is used to determine the three-dimensional structure of the molecule in the crystal. However, in the absence alone of a suitable molecular model, this cannot be done from a single measurement of reflection intensities because certain

information, known as phase information, is lost between the three-dimensional shape of the molecule and its Fourier transform, the diffraction pattern. This phase information must be acquired by methods described below in order to perform a Fourier transform on the diffraction pattern to obtain the three-dimensional structure of the molecule in the crystal. It is the determination of phase information that in effect refocuses X-rays to produce the image of the molecule.

One method of obtaining phase information is by isomorphous replacement, in which heavy-atom derivative crystals are used. In this method, the positions of heavy atoms bound to the molecules in the heavy-atom derivative crystal are determined, and this information is then used to obtain the phase information necessary to elucidate the three-dimensional structure of a native crystal. (Blundel et al., 1976, Protein Crystallography, Academic Press).

Another method of obtaining phase information is by molecular replacement, which is a method of calculating initial phases for a new crystal of a polypeptide or polypeptide co-complex whose structure coordinates are unknown by orienting and positioning a related polypeptide whose structure coordinates are known within the unit cell of the new crystal so as to best account for the observed diffraction pattern of the new crystal. To enable this, the related molecule must have a similar three dimensional structure. Briefly, the principle behind the method of molecular replacement is as follows. A suitable search model, whose three-dimensional structure is similar to that of the unknown target, is identified first. The search model is then rotated and translated within the unit cell of the unknown. For each position of the model, a set of structure factors of the model is computed. These calculated structure factors are then compared with the measured intensities of the unknown and expressed as correlation coefficients. The solution with the highest correlation coefficient is selected as the true solution. These concepts are discussed at length in the book "The Molecular Replacement Method edited by Rossmann (1972, Int. Sci. Rev. Ser. No 13, Gordon & Breach, New York).

A third method of phase determination is multi-wavelength anomalous dispersion or MAD. In this method, X-ray diffraction data are collected at several different wavelengths from a single crystal containing at least one heavy atom with

absorption edges near the energy of incoming X-ray radiation. The resonance between X-rays and electron orbitals leads to differences in X-ray scattering that permits the locations of the heavy atoms to be identified, which in turn provides phase information for a crystal of a polypeptide. A detailed discussion of MAD analysis can be found in Hendrickson, 1985, Trans. Am. Crystallogr. Assoc., 21:11; Hendrickson et al., 1990, EMBO J. 9:1665; and Hendrickson, 1991, Science 4:91.

A fourth method of determining phase information is single wavelength anomalous w dispersion or SAD. In this technique, X-ray diffraction data are collected at a single wavelength from a single native or heavy-atom derivative crystal, and phase information is extracted using anomalous scattering information from atoms such as sulfur or chlorine in the native crystal or from the heavy atoms in the heavy-atom derivative crystal. A detailed discussion of SAD analysis can be found in Brodersen et al., 2000, Acta Cryst., D56:431-441.

A fifth method of determining phase information is single isomorphous replacement with anomalous scattering or SIRAS. This technique combines isomorphous replacement and anomalous scattering techniques to provide phase information for a crystal of a polypeptide. X-ray diffraction data are collected at a single wavelength, usually from a single heavy-atom derivative crystal. Phase information obtained only from the location of the heavy atoms in a single heavy-atom derivative crystal leads to an ambiguity in the phase angle, which is resolved using anomalous scattering from the heavy atoms. Phase information is therefore extracted from both the location of the heavy atoms and from anomalous scattering of the heavy atoms. A detailed discussion of SIRAS analysis can be found in North, 1965, Acta Cryst. 18:212-216; Matthews, 1966, Acta Cryst. 20:82-86.

Once phase information is obtained, it is combined with the diffraction data to produce an electron density map, an image of the electron clouds that surround the molecules in the unit cell. The higher the resolution of the data, the more distinguishable are the features of the electron density map, e.g., amino acid side chains and the positions of carbonyl oxygen atoms in the peptide backbones, because atoms that are closer together are resolvable. A model of the macromolecule is then built into the electron density map with the aid of a computer,

using as a guide all available information, such as the polypeptide sequence and the established rules of molecular structure and stereochemistry. Interpreting the electron density map is a process of finding the chemically realistic conformation that fits the map precisely.

After a model is generated, the structure is refined. Refinement is the process of minimizing the function Φ, which is the difference between observed and calculated intensity values (measured by an R-factor), and which is a function of the position, temperature factor, and occupancy of each non-hydrogen atom in the model. This usually involves alternate cycles of real space refinement, i.e., calculation of electron density maps and model building, and reciprocal space refinement, i.e., computational attempts to improve the agreement between the original intensity data and intensity data generated from each successive model. Refinement ends when the function Φ converges on a minimum wherein the model fits the electron density map and is stereochemically and conformationally reasonable. During refinement, ordered solvent molecules are added to the structure.

d. Various representations

The atomic structure coordinates and machine readable media of the application have a variety of uses. The present invention encompasses the structure coordinates and other information, e.g., amino acid sequence, connectivity tables, vector-based representations, temperature factors, etc., used to generate the three-dimensional structures of the polypeptides for use in the software programs described below and other software programs. For example, the coordinates listed in Table 3 (Figure 25) are useful for solving the three-dimensional crystal or solution structures of other proteins to high resolution.

Additionally, the invention encompasses machine readable media embedded with the three-dimensional structures of the models described herein, or with portions thereof. As used herein, "machine readable medium" or "computer readable medium" refers to any medium that can be read and accessed directly by a computer or scanner. Such media include, but are not limited to: magnetic storage

media, such as floppy discs, hard disc storage medium and magnetic tape; optical storage media such as optical discs or CD-ROM; electrical storage media such as RAM or ROM; and hybrids of these categories such as magnetic/optical storage media. Such media further include paper on which is recorded a representation of the atomic structure coordinates, e.g., Cartesian coordinates, that can be read by a scanning device and converted into a three-dimensional structure with an Optical Character Recognition (OCR).

A variety of data storage structures are available to a skilled artisan for creating a computer readable medium having recorded thereon the atomic structure coordinates of the application or portions thereof and/or X-ray diffraction data. The choice of the data storage structure will generally be based on the means chosen to access the stored information. In addition, a variety of data processor programs and formats can be used to store the sequence and X-ray data information on a computer readable medium. Such formats include, but are not limited to, Protein Data Bank ("PDB") format (Research Collaboratory for Structural Bioinformatics; http://www.rcsb.org/pdb/docs/format/pdbguide2.2/guide2.2_frame.html); Cambridge Crystallographic Data Centre format (http://www.ccdc.cam.ac.uk/support/csd_doc/volume3/z323.html); Structure-data ("SD") file format (MDL Information Systems, Inc.; Dalby et al., 1992, J. Chem. Inf. Comp. Sci. 32:244-255), and line-notation, e.g., as used in SMILES (Weininger, 1988, J. Chem. Inf. Comp. Sci. 28:31-36). Methods of converting between various formats read by different computer software will be readily apparent to those of skill in the art, e.g., BABEL (v. 1.06, Walters & Stahl, © 1992, 1993, 1994; http://www.brunel.ac.uk/departments/chem/babel.htm.) All format representations of the polypeptide coordinates described herein, or portions thereof, are contemplated by the present invention. By providing computer readable medium having stored thereon the atomic coordinates of the application, one of skill in the art can routinely access the atomic coordinates of the application, or portions thereof, and related information for use in modeling and design programs, described in detail below.

While Cartesian coordinates are important and convenient representations of the three-dimensional structure of a polypeptide, those of skill in the art will readily recognize that other representations of the structure are also useful. Therefore, the three-dimensional structure of a polypeptide, as discussed herein, includes not only the Cartesian coordinate representation, but also all alternative representations of the three-dimensional distribution of atoms. For example, atomic coordinates may be represented as a Z-matrix, wherein a first atom of the protein is chosen, a second atom is placed at a defined distance from the first atom, a third atom is placed at a defined distance from the second atom so that it makes a defined angle with the first atom. Each subsequent atom is placed at a defined distance from a previously placed atom with a specified angle with respect to the third atom, and at a specified torsion angle with respect to a fourth atom. Atomic coordinates may also be represented as a Patterson function, wherein all interatomic vectors are drawn and are then placed with their tails at the origin. This representation is particularly useful for locating heavy atoms in a unit cell. In addition, atomic coordinates may be represented as a series of vectors having magnitude and direction and drawn from a chosen origin to each atom in the polypeptide structure. Furthermore, the positions of atoms in a three-dimensional structure may be represented as fractions of the unit cell (fractional coordinates), or in spherical polar coordinates.

Additional information, such as thermal parameters, which measure the motion of each atom in the structure, chain identifiers, which identify the particular chain of a multi-chain protein or protein co-complex in which an atom is located, and connectivity information, which indicates to which atoms a particular atom is bonded, is also useful for representing a three-dimensional molecular structure.

e. Structure of Argonaute

The present invention provides high-resolution three-dimensional structures and atomic structure coordinates of crystalline Argonaute as determined by X-ray crystallography. The specific methods used to obtain the structure coordinates are provided in the examples and throughout the application. The atomic structure coordinates of crystalline Argonaute are listed in Table 3 (Figure 25).

Those having skill in the art will recognize that atomic structure coordinates as determined by X-ray crystallography are not without error. Thus, it is to be understood that any set of structure coordinates obtained for crystals of Argonaute, whether native crystals, derivative crystals or co-crystals, that have a root mean square deviation ("r.m.s.d.") of less than or equal to about 1.5 Angstrom when superimposed, using backbone atoms (N, Cα, C and O), on the structure coordinates listed in Table 3 (Figure 25) are considered to be identical with the structure coordinates listed in the Table 3 (Figure 25) when at least about 50% to 100% of the backbone atoms of Argonaute are included in the superposition.

II. Crystalline Argonaute

It is to be understood that the crystalline Argonaute of the application are not limited to naturally occurring or native Argonaute. Indeed, the crystals of the application include crystals of mutants of native Argonaute. Mutants of naturally-occurring or native Argonautes are obtained by replacing at least one amino acid residue in a native Argonaute with a different amino acid residue, or by adding or deleting amino acid residues within the native polypeptide or at the N- or C-terminus of the native polypeptide, and have substantially the same three-dimensional structure as the native Argonaute from which the mutant is derived.

By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates that have a root-mean-square deviation of less than or equal to about 2 angstrom when superimposed with the atomic structure coordinates of the native Argonaute from which the mutant is derived when at least about 50% to 100% of the Ca atoms of the native Argonaute domain are included in the superposition.

Amino acid substitutions, deletions and additions which do not significantly interfere with the three-dimensional structure of the Argonaute will depend, in part, on the region of the Argonaute where the substitution, addition or deletion occurs. In highly variable regions of the molecule, non-conservative substitutions as well as conservative substitutions may be tolerated without significantly disrupting the three-dimensional, structure of the molecule. In highly conserved regions, or

regions containing significant secondary structure, conservative amino acid substitutions are preferred.

Conservative amino acid substitutions are well known in the art, and include substitutions made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity and/or the amphipathic nature of the amino acid residues involved. For example, negatively charged amino acids include aspartic acid and glutamic acid; positively charged amino acids include lysine and arginine; amino acids with uncharged polar head groups having similar hydrophilicity values include the following: leucine, isoleucine, valine; glycine, alanine; asparagine, glutamine; serine, threonine; phenylalanine, tyrosine. Other conservative amino acid substitutions are well known in the art.

For Argonaute obtained in whole or in part by chemical synthesis, the selection of amino acids available for substitution or addition is not limited to the genetically encoded amino acids. Indeed, the mutants described herein may contain non-genetically encoded amino acids. Conservative amino acid substitutions for many of the commonly known non-genetically encoded amino acids are well known in the art. Conservative substitutions for other amino acids can be determined based on their physical properties as compared to the properties of the genetically encoded amino acids.

In some instances, it may be particularly advantageous or convenient to substitute, delete and/or add amino acid residues to a native Argonaute in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the polypeptide, and for crystallization of the polypeptide. Such substitutions, deletions and/or additions which do not substantially alter the three dimensional structure of the native Argonaute domain will be apparent to those of ordinary skill in the art.

It should be noted that the mutants contemplated herein need not all exhibit Argonaute activity. Indeed, amino acid substitutions, additions or deletions that interfere with the Argonaute activity but which do not significantly alter the three-dimensional structure of the domain are specifically contemplated by the invention.

Such crystalline polypeptides, or the atomic structure coordinates obtained therefrom, can be used to identify compounds that bind to the native domain. These compounds can affect the activity of the native domain.

The co-crystals of the application generally comprise a crystalline Argonaute domain polypeptide in association with one or more compounds. The association may be covalent or non-covalent. Such compounds include, but are not limited to, cofactors, substrates, substrate analogues, modulators, allosteric effectors, etc.

Argonaute

As used herein, the term "Argonaut" refers to a protein which (a) mediates an RNAi response and (b) has an amino acid sequence at least 50 percent identical, and more preferably at least 75, 85, 90 or 95 percent identical to SEQ ID NOs.: 1-5.

Mammals contain four Argonaute1 subfamily members, Ago1-Ago4 (nomenclature as in (Carmell et al., Genes Dev. 16, 2733 (2002)), see Fig. 22 which provides sequence alignment of human Ago1-4 proteins, corresponding to SEQ ID NOs: 1-4). Different Argonaute family members in Drosophila preferentially associate with different small RNAs, with Ago1 preferring miRNAs and Ago2 siRNAs (24). Recent studies of dmAgo1 and dmAgo2 mutants have strengthened these conclusions (25). To assess whether mammalian Ago proteins specialized in their interactions with small RNAs, Ago-associated miRNA populations were examined by microarray analysis (Example 1).

Amino Acid Sequence of *Pyrococcus furiosus* Argonaute Protein:

SEQ ID NO.: 5

MKAKVVINLVKINKKIIPDKIYVYRLFNDPEEELQKEGYSIYRLAYEN
VGIVIDPENLIIATTKELEYEGEFIPEGEISFSELRNDYQSKLVLRLLKENGIGE
YELSKLLRKFRKPKIFGDYKVIPSVEMSVIKHDEDFYLVIHIIHQIQSMKTLW
ELVNKDPKELEEFLMTHKENLMLKDIASPLKTVYKPCFEEYTKKPKLDHNQ
EIVKYWYNYHIERYWNTPEAKLEFYRKFGQVDLKQPAILAKFASKIKKNKN
YKIYLLPQLVVPTYNAEQLESDVAKEILEYTKLMPEERKELLENILAEVDSDI

IDKSLSEIEVEKIAQELENKIRVRDDKGNSVPISQLNVQKSQLLLWTNYSRKY
PVILPYEVPEKFRKIREIPMFIILDSGLLADIQNFATNEFRELVKSMYYSLAKK
YNSLAKKARSTNEIGLPFLDFRGKEKVITEDLNSDKGIIEVVEQVSSFMKGKE
LGLAFIAARNKLSSEKFEEIKRRLFNLNVISQVVNEDTLKNKRDKYDRNRLD
LFVRHNLLFQVLSKLGVKYYVLDYRFNYDYIIGIDVAPMKRSEGYIGGSAV
MFDSQGYIRKIVPIKIGEQRGESVDMNEFFKEMVDKFKEFNIKLDNKKILLLR
DGRITNNEEEGLKYISEMFDIEVVTMDVIKNHPVRAFANMKMYFNLGGAIY
LIPHKLKQAKGTPIPIKLAKKRIIKNGKVEKQSITRQDVLDIFILTRLNYGSISA
DMRLPAPVHYAHKFANAIRNEWKIKEEFLAEGFLYFV

1. Overall Architecture

This application provides the structure of the full-length Argonaute from the archaebacterium *Pyrococcus furiosus* (PfAgo) as determined by x-ray crystallography to 2.25 Å resolution. The structure was solved by multiple anomalous dispersion (MAD) and isomorphous replacement using selenium and mercury derivatives (Table 2 shown in Figure 24)). The N-terminal, middle, and PIWI domains form a crescent-shaped base, with the PIWI domain at the center of the crescent. The region following the N-terminus forms a "stalk" that holds the PAZ domain above the crescent and an interdomain connector cradles the molecule (Fig. 1). This architecture results in a cleft formed at the center of the crescent with the PAZ domain closing in on this cleft.

The N-terminal domain consists of a long strand at the bottom of the crescent, continuing to a region of a small four-stranded β-sheet, three α-helices and a β-hairpin, which then extends to the three-stranded antiparallel β-sheet stalk.

Also provided is the PAZ domain, a globular domain that adopts an OB-like β-barrel fold with an attachment on one side of the barrel and a cleft in between. This cleft was shown to be the binding site for the 2-nucleotide 3'-overhang of the siRNA (29, 32, 33) and is angled towards the crescent. The PAZ domain in PfAgo superimposes very well with the PAZ domains from Drosophila Argonaute 1 (30) and 2 (29, 31) and with the human Argonaute-1 (hAgo1) PAZ domain in complex

with a "mini-siRNA" (33), though the attachment in the archael protein has two α-helices rather than an α-helix and a β-hairpin (Figs. 2A and 2B).

The middle domain, which is located at one end of the crescent, is an α/β open sheet domain composed of a central three-stranded parallel β-sheet surrounded by α-helices. This domain is similar to the glucose-galactose-arabinose-ribose binding protein family and is most similar to Lac repressor (35). The middle domain also has small three-stranded β-sheet on the outer surface of the crescent, connecting it to the rest of the molecule.

Further provided is the PIWI domain, which is at the C-terminus of Argonaute (residues 545-770). It sits in the middle of the crescent and below the PAZ domain. The crystal structure reveals the presence of a prominent central five-stranded β-sheet flanked on both sides by α-helices at the core of the PIWI domain. A smaller β-sheet extends from the central β-sheet and attaches PIWI to the N-terminal domain and to portions of the interdomain connector.

2. Domain Structure

As mentioned above, the PAZ domain superimposes very well with all the other PAZ domains with known structures, namely, Drosophila Argonautes 1 and 2 and hAgo1 (Fig. 2A). Most of the differences lie in loop regions. The root-mean-square deviation (rmsd) between hAgo1-PAZ and the PAZ domain in this structure is approximately 1.4 Å (for 53 Ca's). Though it is now possible to align the sequence of the PAZ domain of PfAgo with PAZ domains from Argonaute proteins of higher eukaryotes (Fig. 2B) based on the structures, homologies between the archeal and eukaryotic PAZ domains was not apparent before the PfAgo structure was determined. In fact, primary sequence comparisons provided no evidence that PfAgo contained a PAZ domain. Even after attempting to align the sequences with reference to the three-dimensional structures, the sequence identity remains below 10%. The presence and location of the PIWI domain was, on the other hand, obvious from the primary sequence, and could be readily identified through BLAST searches.

The role of the PAZ domain, as shown for fly Ago-2 (29, 32) and for hAgo-1 (33) is to bind the 2-nucleotide 3' overhang of the siRNA. Importantly, the conserved aromatic residues that fill the cleft and were shown to bind those nucleotides (29, 32, 33) are all present in the PfAgo PAZ domain. Curiously, in some cases, these side chains occupy similar positions in space even if they aren't anchored to positions on the peptide backbone corresponding to those in eukaryotic proteins. Specifically, Y212, Y216, H217 and Y190 are equivalent to Y309, Y314, H269 and Y277 of hAgo1 that were shown to bind the oxygens of the phosphate that links the two bases in the overhang. Residue Y190 of PfAgo superimposes perfectly on hAgo1-Y277 that was also shown to bind the 2'-hydroxyl of the penultimate nucleotide. Residues L263 and I261 can assume the role of L337 and T335, which anchor the sugar ring of the terminal residue through van der Waals interactions in the hAgo1-RNA structure. There is an aromatic residue, F292 in hAgo1 that stacks against the terminal nucleotide. This position is occupied by another aromatic, W213, in PfAgo. Finally, R220 in the structure of the present application is positioned similarly to K313 that contacts the penultimate nucleotide. As for residues that were shown to bind the region of the RNA strand 5' to the overhang, K191 is positioned as R278 in hAgo1 to bind phosphates and Y259 is equivalent to K333. Other PAZ residues, such as K252, K248, Q276 and N176 are probably used to bind that strand as well. Accordingly, the PAZ domain in PfAgo appears to have a similar function to the PAZ domains of the fly and human Argonautes and would also be capable of binding a 3' single-stranded region of an RNA molecule.

The present application also provides a PIWI domain core having a tertiary structure that belongs to the RNase H family of enzymes, which include RNase H type 1 and type 2 enzymes. This fold is also characteristic of other enzymes with nuclease or polynucleotidyl transferase activities, such as HIV and ASV integrases (36, 37), RuvC (38), a Holliday junction endonuclease, and transposases such as Mu (39) and Tn5 (40). The closest matches, however, are with RNase HII (41) and RNase H1 (42). The rmsd's between these proteins and PfAgo are of 1.9 Å and they are topologically identical (Fig. 3A). RNase H fold proteins all have a five-stranded mixed β-sheet surrounded by helices. In the RNase H enzymes as well as PIWI, there are two helices on either side of the β-sheet. On one side these are very

similar, and on the other, one of the helices varies. PIWI has an insertion between the last strand and the last helix of the RNase H fold. This insertion consists of a smaller β-sheet attachment and a helix that links it to the rest of the protein. RNase HII has a cap domain that sits above the active site cleft and forms a groove for substrate binding (43). In addition, several residues from the cap domain appear to participate in substrate recognition. The positioning of the cap relative to the RNase H fold of the protein is approximately the same as the PAZ domain relative to the PIWI domain in Argonaute.

Similarity is not restricted to the protein fold. In all of these enzymes there are three highly conserved carboxylates which are essential for catalytic activity (44). Two of these carboxylate side chains are always located on the first strand, β1, which is the central strand of the β-sheet, and at the C-terminus of the fourth strand, β4, of the RNase H fold, which is adjacent to β1 (the red and green strands in Figs. 3A and 3B). The position of the third carboxylate varies between the different RNase H fold enzymes. Remarkably, when examining a superposition between either RNase H1 or RNase HII and PIWI, two aspartate residues were located at the same positions as the invariant carboxylates of the RNase H fold (Fig. 3B). These are D558 located on the first b-strand of PIWI and D628 located at the end of the fourth strand of the PIWI domain. These aspartates are equivalent to D10 and D70 in *E. coli* RNase H1, D7 and D112 in *Methanococcus jannaschii* RNase HII, and D6 and D101 in *Archaeoglobus fulgidus* RNase HII. The location of the third carboxylate, a glutamate, in RNase H1 and HII is occupied by a valine in Argonaute. However, a glutamate, E635, is in close proximity to the two aspartates, and this glutamate may serve as the third active site residue. This residue is positioned on the second helix of the RNase H fold of PIWI (the blue helix in Figs. 3A-3B). Since the position of the third carboxylate varies in these proteins, the only requirement would be for a reasonable spatial position at the active site, a criterion which E635 meets. Therefore, the active site of PfAgo is likely composed of the carboxylate triad formed by D528, D628 and E635 that make up the "DDE" motif. Interestingly, an arginine, R627, is also positioned at the center of the active site, as in the case of the IS4 family of transposases such as Tn5 which appear to have a "DDRE motif"

(40, 45). The active site is thus positioned in a cleft in the middle of the crescent in the groove below the PAZ domain.

RNase H enzymes as well as other polynucleotidyl transferase enzymes require the presence of divalent metal ions for activity. However, the precise role of the metal ions remains unclear. Both one and two metal ion mechanisms have been proposed. *E. coli* RNase H1 is thought to work via a one-metal ion mechanism in which Mg^{2+}, coordinated by one carboxylate group, mediates interactions with the nucleic acid substrate. The other two carboxylates activate a water molecule that can then attack the scissile phosphate bond (46, 47). The two-metal ion mechanism was first proposed for the 3' to 5' exonuclease of the Klenow fragment (48, 49). In this case, one metal interacts with the substrate and stabilizes the reaction intermediate and the other activates a water molecule and positions it to attack the scissile phosphate. Indeed, only one metal is observed in the crystal structures of *E. coli* RNase H1 (42) and *A. fulgidus* RNase HII (43) while two are seen in the active site of the isolated HIV RNase H domain of reverse transcriptase (50). Though the absence of a second metal ion in a crystal structure does not preclude a two-metal ion mechanism (since the second metal may have weak binding in the absence of substrates) there are indications that RNase H1 does use a single-metal ion mechanism while HIV RNase H uses two (51). For the PIWI domain of PfAgo, a strong peak is identified in the F_{obs}-F_{calc} difference electron density map near D558, and it is assigned as a water molecule at this time. By growing crystals in the presence of divalent metal ions, this may be assigned as a metal site unambiguously. A divalent metal ion appears to be required for Argonaute activity (52, 53).

3. siRNA Binding

The role of Argonaute is presently unknown in archaebacteria. Because of its similarity to Argonautes in eukaryotes, the siRNA binding characteristics of PfAgo were examined by using crosslinking and competition assays. A single-stranded 21-mer siRNA containing an IodoU nucleotide to facilitate crosslinking gave rise to a crosslinked species, whereas a double-stranded siRNA did not (Fig. 4A). In addition, the same labeled ss-siRNA can be readily competed off with an identical unlabeled oligonucleotide. However, a similar ss-siRNA lacking the 5'-

phosphate moiety was unable to compete for crosslinking, even at greater than ten-fold the concentration than that at which competition with the 5'-phosphorylated ss-siRNA was seen (Fig. 4B). Thus, there appears to be a requirement for a bona fide siRNA for binding. Preferential binding of the ss-siRNA over the ds-version is consistent with the observation that a ds-siRNA cannot be loaded in vitro to an RISC complex, though an ss-siRNA can be. Accordingly, the present application provides an RISC complex comprising an RNAi construct, e.g., an ss-siRNA. The RISC complex preferably comprises an Argonaute protein, most preferably, an Argonaute protein with the "slicer" activity, described in greater detail below.

4. "Slicer" Activity

The finding that the PIWI domain in Argonaute is an RNase H domain suggests Argonaute as the, as of yet unidentified, "Slicer" enzyme of RISC, that is, the enzyme that cleaves the mRNA. RNase H enzymes specialize in single-stranded cleavage of RNA "guided" by a DNA strand in a double-stranded RNA/DNA hybrid. In a similar manner, Argonautes may specialize in RNA cleavage, in particular mRNA, guided by the siRNA strand in a ds RNA substrate. Moreover, unlike most RNases that leave a 3'-phosphate and 5'-OH, RNase H enzymes produce products with 3'-OH and 5' phosphate groups (54). Recently, Martinez and Tuschl, and Zamore and colleagues showed that cleavage of the mRNA by RISC produces the latter type of termini (52, 53). A dependence on Mg^{2+} for activity is another hallmark of RNase H enzymes and RISC was also shown to require Mg^{2+} for cleavage as well (52). The PAZ domain, shown to recognize and bind the 3' ends of siRNAs, and the PIWI domain, now shown to be an RNase H domain for catalytic activity, combine the necessary features of the slicing component of the RNAi machinery. Therefore, Argonaute, the signature component of RISC, can be "Slicer" itself.

5. A Model for si-RNA-Guided mRNA Cleavage

The placement of the PAZ domain on top of the crescent formed by the N-terminal, middle and PIWI domains and cradled by the connecter region in the structure of Argonaute defines a distinct groove through the protein. The groove has

a claw shape that bends around between the PAZ and N-terminal domains. A striking feature of the structure is evident when the electrostatic potential is mapped on the surface of the protein. As shown in Fig. 5A, the surface of this inner groove is completely lined with positive charges. These positive charges are of course suitable for interaction with the negatively charged phosphate backbone and with the 2'-hydroxyl moieties of an RNA molecule, implicating the groove for substrate binding. The substrate for Argonaute is a ds-RNA molecule composed of an ss-siRNA acting as a guide and the mRNA.

In order to examine possible substrate binding modes for Argonaute, the knowledge of siRNA binding to the PAZ domain using the known PAZ-RNA structure (33) and the mode of binding of RNase H substrates (43, 55-57) were combined. Since the PAZ domain of PfAgo superimposes so well with the PAZ domain of hAgo1 in the PAZ-RNA complex as shown above, the two PAZ domains were superimposed and examined for the resulting position of the RNA with respect to PfAgo. The strand that interacts with its 3' end in the PAZ cleft was regarded as the siRNA guide. The second strand would then be regarded as the mRNA substrate strand (see Fig. 5B). The siRNA guide has its 2 nucleotides at its 3' end inserted into the PAZ cleft. The nucleotides just 5' to that track the top of the PAZ b-barrel making very similar, if not identical, interactions with the PAZ domain as in the crystal structure of the PAZ-RNA complex. A long loop present in the PfAgo PAZ domain would probably move up slightly to accommodate the siRNA. Upon examination of the resulting location of the passenger strand, the mRNA would be coming into the binding groove with its 5' end between the PAZ and the N- terminal domains. The N-terminus then acts as an "mRNA grip" on that end of the molecule. It should be noted that there is another extension of the groove that lies between the N-terminal and the PIWI domains, which could accommodate a single-stranded nucleic acid.

The double-stranded RNA was further extended into the molecule along the binding groove by model building. Remarkably, the mRNA would be positioned above the active site located in the PIWI domain 9 nucleotides from the 5'-side end of the double-stranded region, or rather 11 nucleotides if the 2 nucleotides of the

guide that are inserted into the PAZ domain are counted and are probably not interacting with the mRNA. In other words, the scissile bond would be predicted to be between nucleotides 11 and 12 from the 5' end of the message or from the 3'-end of the guide. This precisely coincides with the demonstrated cleavage of mRNAs by RISC 10 nucleotides from the 5' end of an siRNA. The remainder of the RNA would then continue along the binding groove (Fig. 5C). The interdomain connecter is also forming part of the back wall of the binding groove. As the RNA molecule would have to bend somewhat, the details of some of these interactions are not clear. However, the length of the groove appears to accommodate the length of the siRNA guide, with the 5' end of the guide probably interacting with the other side of the groove. From studies of other RNase H enzymes, Argonaute may sense the minor groove width of the dsRNA, which is different from that of dsDNA and from the minor groove width of a RNA/DNA hybrid, and which is in accord with the inability of RISC to cut DNA substrates (53). This mode of recognition would be in addition to binding the 3' end of the siRNA and sensing the phosphate at the 5'end, as shown in the binding experiments (Fig. 4).

The groove as observed in the crystal structure presented here, in the absence of substrate, would fit an A-RNA double helix snugly. Though a single-stranded RNA should bind fairly readily, opening the claw of the molecule somewhat might assist binding the mRNA, after which it can close down on the double stranded substrate. A hinge region may exist in the interdomain connector at residues 317-320. This hinge could lift the PAZ and the away from the crescent base. This is reasonable since a RISC loading complex appears to be required for assembling an active RISC (58, 59).

The notion that RISC "Slicer" activity, i.e. siRNA-guided mRNA cleavage, resides in Argonaute itself was tested in a mammalian system where the RNAi pathway is known to function. It appears that mammalian Argonaute proteins are distinct and that Ago2 is functional for mRNA cleavage. Based on the sequence alignment with the archael protein, D597, D669 and a third amino acid (e.g., E683) of hAgo2 correspond to D558, D628 and E635 of PfAgo to form the catalytic triad "DDE" motif. There is an insertion near E683, and E673 may also act as the third

carboxylate in hAgo2. The conserved active site aspartates were mutated and the mutants lost their nuclease activity while retaining binding to the siRNA guide. Therefore, Argonaute itself functions as the Slicer enzyme in the RNAi pathway.

In siRNA-guided mRNA cleavage, once RISC is formed, it needs to identify its homologous targets, both for target cleavage and for repression at the level of protein synthesis. In the latter case, there is a presumably stable interaction that occurs between the siRNA and its target, with the target being somehow protected from cleavage. Certainly, an absence of base pairing in the region of the active site might distort the complex sufficiently to prevent catalysis.

Furthermore, several Argonaute protein family members appear to be inactive towards mRNA cleavage despite the presence of the catalytic residues. The basis for these differences may help elucidate the details of the mechanism for siRNA-guided mRNA cleavage. The situation here might be somewhat analogous to the case of the transposase Tn5 and its inhibitor, which posses a catalytic domain with a similar RNase H-like fold. Tn5 inhibitor is a truncated version of the active Tn5 transposase and retains the essential catalytic residues. However, there are major conformational differences between the two that result in domains of the proteins being in different positions relative to one another (40, 45). Similarly, mutations have been introduced into a catalytically active Ago protein, hAgo2, in the vicinity of the active site, which change residues to corresponding residues in an inactive Ago, hAgo1. These inactivate Ago2 for cleavage, indicating that there are determinants for catalysis beyond simply the catalytic triad and that relatively minor alterations in the PIWI domain can have profound effects on its activity toward RNA substrates. The common fold in the catalytic domain of Argonaute family members and transposases and integrases is also intriguing given the relationship of RNAi with control of transposition. It is worth noting that the identification of the catalytic center of RISC awaited a drive toward understanding RNAi at a structural level. Thus, it seems likely that, as in the present example, a full understanding of the underlying mechanism of RNAi will derive from a combination of detailed biochemical and structural studies of RISC.

Assays

The assays and methods described herein may used in combination or separately. For example, an in silico screening and an in vitro binding assay and/or an activity assay may be combined to identify a binding agent and/or a binding agent for a protein that also modulates activity of the protein.

I. Assays Based on the Atomic Structure Coordinates

Structural information, often in the form of atomic structure coordinates, may also be used in a variety of molecular modeling and computer-based screening applications to, for example, design variants that have altered biological properties or to computationally design, screen for and/or identify compounds that bind to the Argonaute protein or to fragments of the Argonaute protein. These compounds may modulate the activity of Argonaute protein and hence the RISC activity.

Thus, in a further aspect of the application, the data from the crystal structure of Argonaute is used to evaluate compounds for their utility as modulators of Argonuate protein. These methods comprise designing and synthesizing candidate compounds using the atomic coordinates of the three dimensional structure of such co-crystals and screening for its utility in various pharmaceutical applications.

In another embodiment, the structures are probed with a plurality of molecules to determine their ability to bind to the Argonaute protein at various sites. Such molecules may be able to modulate the activity of Argonaute protein.

In yet another embodiment, the structures can be used to computationally screen small molecule databases for chemical entities or compounds that can bind in whole, or in part, to Argonaute. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy. (Meng et al., 1992, J. Comp. Chem. 13:505-524).

The design of compounds that bind to Argonaute according to this invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with Argonaute. This association

can be covalent or non-covalent. For example, covalent interactions may be important for designing suicide or irreversible inhibitors of a protein. Non-covalent molecular interactions important in the association of Argonaute include hydrogen bonding, ionic and other polar interactions, interactions as well as van der Waals interactions. Second, the compound must be able to assume a conformation that allows it to associate with the Argonaute protein. Although certain portions of the compound will not directly participate in this association with the protein, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical group or compound in relation to all or a portion of the binding site, or the spacing between functional groups of a compound comprising several chemical groups that directly interact with the protein.

The potential modulatory or binding effect of a chemical compound on Argonaute may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and the protein, synthesis and testing of the compound is unnecessary. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to the protein and inhibit its activity. In this manner, synthesis of ineffective compounds may be avoided.

A binding compound of Argonaute may be computationally evaluated and designed by means of a series of steps in which chemical groups or fragments are screened and selected for their ability to associate with the individual binding pockets or interface surfaces of each of the proteins. One skilled in the art may use one of several methods to screen chemical groups or fragments for their ability to associate with Argonaute. Docking may be accomplished using software such as QUANTA and SYBYL, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical groups. These include:

1. GRID (Goodford, 1985, J. Med. Chem. 28:849-857). GRID is available from Oxford University, Oxford, UK;

2. MCSS (Miranker & Karplus, 1991, Proteins: Structure, Function and Genetics 11:29-34). MCSS is available from Molecular Simulations, Burlington, Mass.;

3. AUTODOCK (Goodsell & Olsen, 1990, Proteins: Structure, Function, and Genetics 8:195-202). AUTODOCK is available from Scripps Research Institute, La Jolla, Calif.;

4. DOCK (Kuntz et al., 1982, J. Mol. Biol. 161:269-288). DOCK is available from University of California, San Francisco, Calif.;

5. FlexE (Clausen H, Buning C, Rarey M and Lengauer T) J. Mol. Biol. (2001) 308, 377-395. FlexE is available from Tripos, St. Louis, Mo.;

6. Glide, Glide is available from Schrodinger, Portland, Oreg.;

7. Gold, Jones et al. J. Mol. Biol. 245, 43-53, 1995;

8. QXP, McMartin C, Bohacek RS. J Comput Aided Mol Des 1997 11:333-44;

9. ICM. (http://www.molsoft.com). Available from Molsoft, San Diego, Calif.; and

10. FlexX. [Sybl, Tripos, St. Louis, Mo

Once suitable chemical groups or fragments have been selected, they can be assembled into a single compound. Assembly may proceed by visual inspection of the relationship of the fragments to each other in the three-dimensional image displayed on a computer screen in relation to the structure coordinates of Argonaute. This would be followed by manual model building using software such as QUANTA or SYBYL.

Useful programs to aid one of skill in the art in connecting the individual chemical groups or fragments include:

1. CAVEAT (Bartlett et al., 1989, 'CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules.' In Molecular Recognition in Chemical and Biological Problems', Special Pub., Royal Chem. Soc. 78:182-196). CAVEAT is available from the University of California, Berkeley, Calif.;

2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif.). This area is reviewed in Martin, 1992, J. Med. Chem. 35:2145-2154); and

3. HOOK (available from Molecular Simulations, Burlington, Mass.).

Instead of proceeding to build a modulator of Argonaute in a step-wise fashion one fragment or chemical group at a time, as described above, Argonaute-binding compounds or modulators may be designed as a whole or 'de novo' using either an empty binding site or the surface of a protein that participates in protein/protein interactions in a co-complex, or optionally including some portion(s) of a known modulator(s). These methods include:

1. LUDI (Bohm, 1992, J. Comp. Aid. Molec. Design 6:61-78). LUDI is available from Molecular Simulations, Inc., San Diego, Calif.;

2. LEGEND (Nishibata & Itai, 1991, Tetrahedron 47:8985). LEGEND is available from Molecular Simulations, Burlington, Mass.; and

3. LeapFrog (available from Tripos, Inc., St. Louis, Mo.).

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., Cohen et al., 1990, J. Med. Chem. 33:883-894. See also, Navia & Murcko, 1992, Current Opinions in Structural Biology 2:202-210.

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to Argonaute may be tested and

optimized by computational evaluation. An effective modulator of Argonaute must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., it must have a small deformation energy of binding). Thus, the most efficient modulators should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mol, preferably, not greater than 7 kcal/mol. Modulators may interact with the protein in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the modulator binds to the protein.

A compound selected or designed for binding to or inhibiting Argonaute may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target protein. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the modulator and the protein when the modulator is bound to it preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include: Gaussian 92, revision C (Frisch, Gaussian, Inc., Pittsburgh, Pa. ©1992); AMBER, version 4.0 (Kollman, University of California at San Francisco, ©1994); QUANTA/CHARMM (Molecular Simulations, Inc., Burlington, Mass., ©1994); and Insight II/Discover (Biosym Technologies Inc., San Diego, Calif., ©1994). These programs may be implemented, for instance, using a computer workstation, as are well-known in the art. Other hardware systems and software packages will be known to those skilled in the art.

The computer-assisted methods for designing a modulator of Argonaute activity can be de novo or based on a candidate compound. An example of a computer-assisted method for designing an modulator of Argonaute activity de novo would thus involve the steps of: (1) supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex comprising at least

a portion of an Argonaute; (2) computationally building a chemical entity represented by a set of structure coordinates; and (3) determining whether the chemical entity is an modulator expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential modulation of Aargonaute activity.

Once an modulator or Argonaute binding compound has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or chemical groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. One of skill in the art will understand that substitutions known in the art to alter conformation should be avoided. Such altered chemical compounds may then be analyzed for efficiency of binding to Argonaute by the same computer methods described in detail above.

An example of such a computer-assisted method for identifying an modulator of Argonaute activity would thus involve (1) supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex comprising at least a portion of an Argonaute or Argonaute-like compound, (2) supplying the computer modeling application with a set of structure coordinates of a chemical entity; and (3) determining whether the chemical entity is an modulator expected to bind to or modulate the molecule or molecular complex.

The structure coordinates of an Argonaute co-complex, or of Argonaute alone, or of portions thereof, are particularly useful to solve the structure of other co-complexes of Argonaute, of mutants, of the Argonaute co-complex further complexed to another molecule, or of the crystalline form of any other protein or protein co-complex with significant amino acid sequence homology to any functional domain of Argonaute.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown co-crystal structure, whether it is another Argonaute co-complex, a mutant, a Argonaute co-complex that is further complexed

to another molecule, or the crystal of some other protein or protein co-complex with significant amino acid sequence homology to any functional domain of one of the proteins in the co-complex crystal, may be determined using phase information from the present Argonaute co-complex structure coordinates. This method will provide an accurate three-dimensional structure for the unknown protein or protein co-complex in the new crystal more quickly and efficiently than attempting to determine such information ab initio.

If an unknown crystal form has the same space group as and similar cell dimensions to the known co-complex crystal form, then the phases derived from the known crystal form can be directly applied to the unknown crystal form, and in turn, an electron density map for the unknown crystal form can be calculated. Difference electron density maps can then be used to examine the differences between the unknown crystal form and the known crystal form. A difference electron density map is a subtraction of one electron density map, e.g., that derived from the known crystal form, from another electron density map, e.g., that derived from the unknown crystal form. Therefore, all similar features of the two electron density maps are eliminated in the subtraction and only the differences between the two structures remain. However, if the space groups and/or cell dimensions of the two crystal forms are different, then this approach will not work and molecular replacement must be used in order to derive phases for the unknown crystal form.

The techniques of X-ray diffraction can be employed in the study of the co-complexes of Argonaute. This information may thus be used to optimize known modulators of Argonaute and more importantly, to design and synthesize novel classes of modulators of Argonaute.

Subsets of the atomic structure coordinates can also be used in any of the above methods. Particularly useful subsets of the coordinates include, but are not limited to, coordinates of single domains, coordinates of residues lining an active site, coordinates of residues that participate in important protein-protein contacts at an interface, and Cα coordinates. For example, the coordinates of one domain of a protein that contains the active site may be used to design modulators that bind to that site, even though the protein is fully described by a larger set of atomic

coordinates. Therefore, as described in detail for the specific embodiments, below, a set of atomic coordinates that define the entire polypeptide chain, although useful for many applications, do not necessarily need to be used for the methods described herein.

II. Assay for Argonaute RNase Activity

The present application provides screening methods for agents that modulate the RNase activity of the Argonaute protein. Applicants have shown that Argonaute has a RNase H domain and acts as the Slicer enzyme of RISC to cleave mRNA bound by a single-stranded siRNA. Thus, the Argonaute activity can be assayed by measuring by any standard techniques in the art for measuring RNase activity. The exemplification provides one such example.

In certain embodiments, the RNase H activity of Argonaute can be measured. For example, WO 04/59012 describes a "Molecular Beacon" Assay for measuring RNase H activity and/or other nuclease-mediated cleavage of nucleic acids. Briefly, the assay detects degradation of a nucleic acid substrate which, preferably, is an RNA substrate that is annealed to at least one region or part of an oligonucleotide probe. In preferred embodiments, the oligonucleotide probe is a DNA probe (e.g., a deoxyoligonucleotide probe), which may also be referred to in the context of this invention as the DNA "substrate" moiety. Typically, both the oligonucleotide probe and the RNA substrate will be oligonucleotide molecules that are between about 10 and about 100 nucleotides in length and may be, e.g., between about 1050 nucleotides in length, more preferably between 15-25 nucleotides length. In preferred embodiments, the oligonucleotide probe is at least 18 nucleotides in length.

Chan et al. describes a capillary electrophoretic assay to measure RNase H activity. See Anal Biochem. 2004 Aug 15;331(2):296-302. Briefly, cleavage of a fluorescein-labeled RNA-DNA heteroduplex was monitored by capillary electrophoresis. This assay was used as a secondary assay to confirm hits from a high-throughput screening program. Since autofluorescent compounds in samples migrated differently from both substrate and product in most cases, the assay was

extremely robust for assaying enzymatic inhibition of such samples, in contrast to a simple well-based approach.

The screening methods may be conducted in a high-throughput fashion using any techniques available in the art. Recently, Parniak et al. described a fluorescence-based high-throughput screening assay for inhibitors of HIV RNase H activity. See Anal Biochem 2003, 322:33-9. Briefly, the assay substrate is an 18-nucleotide 3'-fluorescein-labeled RNA annealed to a complementary 18-nucleotide 5'-Dabcyl-modified DNA. The intact duplex has an extremely low background fluorescent signal and provides up to 50-fold fluorescent signal enhancement following hydrolysis. The size and sequence of the duplex are such that HIV-1 RT-RNase H cuts the RNA strand close to the 3' end. The fluorescein-labeled ribonucleotide fragment readily dissociates from the complementary DNA at room temperature with immediate generation of a fluorescent signal. This assay is rapid, inexpensive, and robust, providing Z' factors of 0.8 and coefficients of variation of about 5%. The assay can be carried out both in real-time (continuous) and in "quench" modes; the latter requires only two addition steps with no washing and is thus suitable for robotic operation. Several chemical libraries totaling more than 106,000 compounds were screened with this assay in approximately 1 month.

Alternatively, McLellan et al. described a nonradioactive, 96-well plate assay designed to be used for high-throughput screening of compounds capable of inhibiting the RNase H activity of HIV-1 reverse transcriptase. See McLellan at al., Biotechniques. 2002 Aug;33(2):424-9. In this method, tRNA is employed as substrate that was labeled with digoxygenin-modified reporter residues. The labeled tRNA was prehybridized with a DNA oligonucleotide that contained a single biotinylated residue at its 5'-terminus to ensure its attachment to streptavidin-coated microplates. The uncleaved, immobilized DNA/tRNA substrate was detected through the use of established ELISA protocols. Incubation with purified HIV-1 reverse transcriptase initiated RNase H degradation and caused a signal reduction to negligible background levels. In contrast, the signal intensity remained unaffected when using an RNase H deficient mutant enzyme. The assay was validated using

the hydrazone derivative BBNH that was previously shown to inhibit RNase H degradation below concentrations of 10 microM.

III. Reporter Gene Assay

The application also provides reporter gene assays. The reporter gene assays may be used to identify agents that modulate (e.g., increase) expression of Argonaute gene(s), e.g., by modulating Argonaute's promoter activity. For example, by operably linking an Argonaute's promoter with a reporter gene, the activity of the promoter can be monitored through monitoring/measuring the expression level of reporter gene. Many reporter gene assays have been developed and known to skilled artisans. Examples include: β-galactosidase assays; β-glucuronidase assays; B-lactamase assays (kits, β-lacatamase FRET substrates or color substrates are commercially available); CAT assays; Dual Reporter assays; GFP Assays; Luciferase Assays; SEAP Assays.

IV. Binding Assay

As described above, in silico screening or assays may be developed to identify a ligand or an inhibitor of interest, such as a ligand or an inhibitor that interacts with an Argonaute protein, e.g., a hAgo-2 protein. A ligand generally refers to a molecule (e.g., a nucleic acid molecule or a non-nucleic acid small molecule) that binds a molecule of interest (e.g., an Argonaute protein of the application). An inhibitor generally refers to a molecule that inhibits the function or activity of its target molecule, e.g., an Argonaute protein of the application.

A variety of assay formats will suffice and, in light of the present disclosure, those not expressly described herein will nevertheless be comprehended by one of ordinary skill in the art. Assay formats which approximate such conditions as formation of protein-based complexes and enzymatic activity may be generated in many different forms, and include assays based on cell-free systems, e.g., purified proteins or cell lysates, as well as cell-based assays which utilize intact cells. Simple binding assays can also be used to detect agents which bind to a protein of the application. Agents to be tested can be produced, for example, by bacteria, yeast

or other organisms (e.g., natural products), produced chemically (e.g., small molecules, including peptidomimetics), or produced recombinantly. In a preferred embodiment, the test agent is a small organic molecule, e.g., other than a peptide or oligonucleotide, having a molecular weight of less than about 6,000 daltons.

In many drug screening programs which test libraries of compounds and natural extracts, high throughput assays are desirable in order to maximize the number of compounds surveyed in a given period of time. Assays of the present application which are performed in cell-free systems, such as may be developed with purified or semi-purified proteins or with lysates, are often preferred as "primary" screens in that they can be generated to permit rapid development and relatively easy detection of an alteration in a molecular target which is mediated by a test compound. Moreover, the effects of cellular toxicity and/or bioavailability of the test compound can be generally ignored in the in vitro system, the assay instead being focused primarily on the effect of the drug on the molecular target as may be manifest in the affinity of the drug to the molecular target and/or changes in enzymatic properties of the molecular target.

In certain embodiments, an Argonaute protein to be used in a binding assay is at least semi-purified proteins. By semi-purified, it is meant that the proteins utilized in the reconstituted mixture have been previously separated from other cellular or viral proteins. For instance, in contrast to cell lysates, the protein involved in the protein-based complex formation are present in the mixture to at least 50% purity relative to all other proteins in the mixture, and more preferably are present at 90-95% purity.

Assaying the protein-based complexes of the application, in the presence or absence of a candidate agent, can be accomplished in any vessel suitable for containing the reactants. Examples include microtitre plates, test tubes, and micro-centrifuge tubes.

In an exemplary binding assay, the agent or compound of interest is contacted with an Argonaute protein. Detection and quantification of the Argonaute protein-based complex (e.g., a co-complex formed by the Argonaute protein and the

compound) provides a means for determining the compound's affinity for the Argonaute protein.

Protein-based complex formation may be detected by a variety of techniques, many of which are effectively described herein. For instance, formation of complexes can be quantitated using, for example, detectably labeled proteins (e.g., radiolabeled, fluorescently labeled, or enzymatically labeled), by immunoassay, or by chromatographic detection. Surface plasmon resonance systems, such as those available from Biacore International AB (Uppsala, Sweden), may also be used to detect binding interactions.

Often, it will be desirable to immobilize the protein to facilitate separation of complexes from uncomplexed forms of agents to be assayed for their binding affinity to a protein, as well as to accommodate automation of the assay. In an illustrative embodiment, a fusion protein can be provided which adds a domain that permits the protein (or a portion of the protein) to be bound to an insoluble matrix. For example, GST-Argonaute (or a portion thereof) fusion proteins can be adsorbed onto glutathione sepharose beads (Sigma Chemical, St. Louis, MO) or glutathione derivatized microtitre plates, which are then combined with test agents, e.g., a radio- or fluorescent-labeled agents, and incubated under conditions conducive to complex formation. Following incubation, the beads are washed to remove any unbound test agents, and the matrix bead-bound label(s) determined directly, or in the supernatant after the complexes are dissociated, e.g., when microtitre plate is used.

RNAi

The term "RNAi construct," as used herein, comprises nucleotides that hybridize under physiological condition to a portion of a target gene and attenuates expression of the target gene. In certain embodiments, the RNAi construct, when introduced into a cell, induces a sequence-specific RNA interference process. The RNAi construct used in the present application may be single-stranded siRNAs (ssRNAs), double-stranded siRNAs (dsRNAs), which includes short "hairpin" RNAs (shRNAs). An RNAi construct used in the present application may be single-stranded siRNAs (ssRNAs), double-stranded siRNAs (dsRNAs), which include

short "hairpin" RNAs (shRNAs). The RNAi construct may comprise one or more strands of polymerized ribonucleotide. It may include modifications to either the phosphate-sugar backbone or the nucleoside. For example, the phosphodiester linkages of natural RNA may be modified to include at least one of a nitrogen or sulfur heteroatom. Modifications in RNA structure may be tailored to allow specific genetic inhibition while avoiding a general panic response in some organisms which is generated by RNAi. Likewise, bases may be modified to block the activity of adenosine deaminase. The RNAi construct may be produced enzymatically or by partial/total organic synthesis, any modified ribonucleotide can be introduced by in vitro enzymatic or organic synthesis.

The RNAi construct may be directly introduced into the cell (i.e., intracellularly); or introduced extracellularly into a cavity, interstitial space, into the circulation of an organism, introduced orally, or may be introduced by bathing an organism in a solution containing RNA. Methods for oral introduction include direct mixing of RNA with food of the organism, as well as engineered approaches in which a species that is used as food is engineered to express an RNA, then fed to the organism to be affected. Physical methods of introducing nucleic acids include injection of an RNA solution directly into the cell or extracellular injection into the organism.

The double-stranded structure may be formed by a single self-complementary RNA strand (shRNA) or two complementary RNA strands. RNA duplex formation may be initiated either inside or outside the cell. The RNA may be introduced in an amount which allows delivery of at least one copy per cell. Higher doses (e.g., at least 5, 10, 100, 500 or 1000 copies per cell) of double-stranded material may yield more effective inhibition; lower doses may also be useful for specific applications. Inhibition is sequence-specific in that nucleotide sequences corresponding to the duplex region of the RNA are targeted for genetic inhibition.

RNAi constructs containing a nucleotide sequences identical to a portion, of either coding or non-coding sequence, of the target gene are preferred for inhibition. RNA sequences with insertions, deletions, and single point mutations relative to the target sequence (ds RNA similar to the target gene) have also been found to be

effective for inhibition. Thus, sequence identity may be optimized by sequence comparison and alignment algorithms known in the art (see Gribskov and Devereux, Sequence Analysis Primer, Stockton Press, 1991, and references cited therein) and calculating the percent difference between the nucleotide sequences by, for example, the Smith-Waterman algorithm as implemented in the BESTFIT software program using default parameters (e.g., University of Wisconsin Genetic Computing Group). Greater than 90% sequence identity, or even 100% sequence identity, between the inhibitory RNA and the portion of the target gene is preferred. Alternatively, the duplex region of the RNA may be defined functionally as a nucleotide sequence that is capable of hybridizing with a portion of the target gene transcript (e.g., 400 mM NaCl, 40 mM PIPES pH 6.4, 1 mM EDTA, 50 °C. or 70 °C. hybridization for 12-16 hours; followed by washing). In certain preferred embodiments, the length of the RNAi is at least 20, 21 or 22 nucleotides in length, e.g., corresponding in size to RNA products produced by Dicer-dependent cleavage. In certain embodiments, the RNAi construct is at least 25, 50, 100, 200, 300 or 400 bases. In certain embodiments, the RNAi construct is 400-800 bases in length.

In certain embodiments, an shRNA construct is designed with about 29 bp helices. Further information on the optimization of shRNA constructs may be found, for example, in the following references: Paddison, et al.. Proc Natl Acad Sci U S A, 2002. 99(3): p. 1443-8; 13. Brummelkamp, et al. Science, 2002. 21: p. 21; Kawasaki, et al. Nucleic Acids Res, 2003. 31(2): p. 700-7; Lee et al. Nat Biotechnol, 2002. 20(5): p. 500-5; Miyagishi, et al. Nat Biotechnol, 2002. 20(5): p. 497-500; Paul., et al., Nat Biotechnol, 2002. 20(5): p. 505-8.

The RNAi construct may be synthesized either in vivo or in vitro. Endogenous RNA polymerase of the cell may mediate transcription in vivo, or cloned RNA polymerase can be used for transcription in vivo or in vitro. For transcription from a transgene in vivo or an expression construct, a regulatory region (e.g., promoter, enhancer, silencer, splice donor and acceptor, polyadenylation) may be used to transcribe the RNAi strand (or strands). Inhibition may be targeted by specific transcription in an organ, tissue, or cell type; stimulation of an environmental condition (e.g., infection, stress, temperature, chemical inducers);

and/or engineering transcription at a developmental stage or age. The RNA strands may or may not be polyadenylated; the RNA strands may or may not be capable of being translated into a polypeptide by a cell's translational apparatus. The RNAi construct may be chemically or enzymatically synthesized by manual or automated reactions. The RNAi construct may be synthesized by a cellular RNA polymerase or a bacteriophage RNA polymerase (e.g., T3, T7, SP6). The use and production of an expression construct are known in the art (see also WO 97/32016; U.S. Pat. Nos. 5,593,874, 5,698,425, 5,712,135, 5,789,214, and 5,804,693; and the references cited therein). If synthesized chemically or by in vitro enzymatic synthesis, the RNA may be purified prior to introduction into the cell. For example, RNA can be purified from a mixture by extraction with a solvent or resin, precipitation, electrophoresis, chromatography or a combination thereof. Alternatively, the RNAi construct may be used with no or a minimum of purification to avoid losses due to sample processing. The RNAi construct may be dried for storage or dissolved in an aqueous solution. The solution may contain buffers or salts to promote annealing, and/or stabilization of the duplex strands.

Physical methods of introducing nucleic acids include injection of a solution containing the RNAi construct, bombardment by particles covered by the RNAi construct, soaking the cell or organism in a solution of the RNA, or electroporation of cell membranes in the presence of the RNAi construct. A viral construct packaged into a viral particle would accomplish both efficient introduction of an expression construct into the cell and transcription of RNAi construct encoded by the expression construct. Other methods known in the art for introducing nucleic acids to cells may be used, such as lipid-mediated carrier transport, chemical mediated transport, such as calcium phosphate, and the like. Thus the RNAi construct may be introduced along with components that perform one or more of the following activities: enhance RNA uptake by the cell, promote annealing of the duplex strands, stabilize the annealed strands, or other-wise increase inhibition of the target gene.

"Inhibition of gene expression" refers to the absence or observable decrease in the level of protein and/or mRNA product from a target gene. "Specificity" refers

to the ability to inhibit the target gene without manifest effects on other genes of the cell. The consequences of inhibition can be confirmed by examination of the outward properties of the cell or organism (as presented below in the examples) or by biochemical techniques such as RNA solution hybridization, nuclease protection, Northern hybridization, reverse transcription, gene expression monitoring with a microarray, antibody binding, enzyme linked immunosorbent assay (ELISA), Western blotting, radioimmunoassay (RIA), other immunoassays, and fluorescence activated cell analysis (FACS). For RNA-mediated inhibition in a cell line or whole organism, gene expression is conveniently assayed by use of a reporter or drug resistance gene whose protein product is easily assayed. Such reporter genes include acetohydroxyacid synthase (AHAS), alkaline phosphatase (AP), beta galactosidase (LacZ), beta glucoronidase (GUS), chloramphenicol acetyltransferase (CAT), green fluorescent protein (GFP), horseradish peroxidase (HRP), luciferase (Luc), nopaline synthase (NOS), octopine synthase (OCS), and derivatives thereof. Multiple selectable markers are available that confer resistance to ampicillin, bleomycin, chloramphenicol, gentamycin, hygromycin, kanamycin, lincomycin, methotrexate, phosphinothricin, puromycin, and tetracyclin.

Depending on the assay, quantitation of the amount of gene expression allows one to determine a degree of inhibition which is greater than 10%, 33%, 50%, 90%, 95% or 99% as compared to a cell not treated according to the present application. As an example, the efficiency of inhibition may be determined by assessing the amount of gene product in the cell: mRNA may be detected with a hybridization probe having a nucleotide sequence outside the region used for the inhibitory double-stranded RNA, or translated polypeptide may be detected with an antibody raised against the polypeptide sequence of that region.

As disclosed herein, the present application is not limited to any type of target gene or nucleotide sequence. In some preferred embodiments, the target gene is an essential gene or a gene which is essential for cell viability. The following classes of possible target genes are listed for illustrative purposes: developmental genes (e.g., adhesion molecules, cyclin kinase inhibitors, Wnt family members, Pax family members, Winged helix family members, Hox family members, cytokines,

lymphokines and their receptors, growth/differentiation factors and their receptors, neurotransmitters and their receptors); oncogenes (e.g., ABLI, BCLI, BCL2, BCL6, CBFA2, CBL, CSFIR, ERBA, ERBB, EBRB2, ETSI, ETS1, ETV6, FGR, FOS, FYN, HCR, HRAS, JUN, KRAS, LCK, LYN, MDM2, MLL, MYB, MYC, MYCLI, MYCN, NRAS, PIM 1, PML, RET, SRC, TALI, TCL3, and YES); tumor suppressor genes (e.g., APC, BRCA1, BRCA2, MADH4, MCC, NF 1, NF2, RB 1, P53, BIM, PUMA and WTI); and enzymes (e.g., ACC synthases and oxidases, ACP desaturases and hydroxylases, ADP-glucose pyrophorylases, ATPases, alcohol dehydrogenases, amylases, amyloglucosidases, catalases, cellulases, chalcone synthases, chitinases, cyclooxygenases, decarboxylases, dextrinases, DNA and RNA polymerases, galactosidases, glucanases, glucose oxidases, granule-bound starch synthases, GTPases, helicases, hemicellulases, integrases, inulinases, invertases, isomerases, kinases, lactases, lipases, lipoxygenases, lysozymes, nopaline synthases, octopine synthases, pectinesterases, peroxidases, phosphatases, phospholipases, phosphorylases, phytases, plant growth regulator synthases, polygalacturonases, proteinases and peptidases, pullanases, recombinases, reverse transcriptases, RUBISCOs, topoisomerases, and xylanases).

The application also provides variations of the methods described herein, wherein gene expression of more than one gene is achieved. This may be achieved for example, by expressing multiple shRNAs, or by designing an shRNA to inhibit the gene expression of two or more genes which share substantial nucleotide sequence identity in a short stretch, preferably at least 90% identity over a length of 20, 22, 25, 27, or 30 nucleotides.

The compositions of the present application may be used to enhance the therapeutic effectiveness of a RNAi therapeutics. Exemplary RNAi therapeutics includes double-stranded ribonucleic acids (dsRNAs) for inhibiting the expression of a K-ras oncogene in a cell for treating pancreatic cancer, described in US20040121348, double-stranded ribonucleic acids (dsRNAs) having nucleotide sequences substantially identical to at least a part of a 3'-untranslated region (3'-UTR) of a (+) strand RNA virus useful for treating hepatitis C infection, described in US20040091457, siRNAs that down-regulate expression of neurite growth

inhibitor receptor, prostaglandin D2 receptor, IkappaB kinase or protein kinase PKR genes, useful for treating cancer and inflammatory disease, described in U.S. Patent Application Publication No. 20030191077.

Furthermore, the crystal structure, the electronic representation, as well as other aspects of the application also relate to a method for identifying, designing, and/or optimizing an RNAi construct or RNAi therapeutic of the application. For example, based on the structure of the PAZ domain, particular the site that may interact with the 3' end of a nucleic acid (e.g., an RNA or a portion of an RNAi construct), the nucleic acid sequence or structure may be designed and/or optimize to increase or decrease the nucleic acid's interaction with the PAZ domain. Similarly, based on the PIWI domain as well as the interface between the PIWI domain and the PAZ domain, an RNAi construct or RNAi therapeutic may be designed and/or optimized. An optimized RNAi therapeutic may have an improved pharmacokinetic and/or pharmacodynamic profile.

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All references cited herein including the numbered references above and others throughout the application are incorporated by reference in their entirety.

EQUIVALENTS

While this invention has been particularly shown above and in the following examples and described with references to preferred embodiments thereof, it will be understood by those skilled in the art that various changes in form and details may be made therein without departing from the scope of the invention encompassed by the appended claims.

EXEMPLIFICATION

Example 1. DNA constructs and site-directed mutagenesis

cDNAs encoding full length human Ago1, Ago2, and Ago3 were generated by RT-PCR from RNAs extracted from 293T, HeLa or S2 cells. Plasmids expressing various Argonaute proteins were made by cloning the cDNAs into a pcDNA3-based myc-epitope tagging vector. Mutations were introduced by site-directed mutagenesis using the QuickChange Kit (Stratagene).

Example 2. Human Cell Culture and transfection

Human 293T cells were cultured in DMEM (10% FBS) in a 37 °C incubator with 5% CO2. Cell transfections were carried out using calcium-phosphate buffer or Mirus TransIT-LT1 transfection reagent. Luciferase GL3 siRNA duplex was purchased from Dharmacon. siRNA transfection was carried out by using Oligofectamine (Invitrogen). Procedures for immunoprecipitation and immunoblotting were described previously (Caudy et al, Genes. Dev. 16, 2491 (2002)). Lysis buffer contained 0.5% NP-40, 150mM NaCl, 2 mM $MgCl_2$, 2mM $CaCl_2$ and 20mM Tris-HCl pH 7.5. Protease inhibitor and DTT (final 2mM) were

added immediately before lysis. The antibody to the myc tag (9E10) was purchased from Neomarker. RNAs associated with the Ago immunocomplexes were isolated using phenol-chloroform/chloroform extraction and ethanol precipitation. RNAs were stained using SYBR Gold from Molecular Probes. Small RNA Northern blotting was carried out as described previously (Caudy et al., *supra*).

Example 3. mRNA Cleavage assays and in vitro reconstitution of RISC activity

Capped and uniformly radiolabeled Luciferase mRNA target was in vitro transcribed using the Riboprobe system from Promega and was purified using PAGE as described previously. The immunoaffinity purified Ago complexes were first resuspended in 10 µl buffer containing 100mM KCl, 2mM $MgCl_2$ and 10mM Tris pH7.5. For in vitro reconstitution of RISC activity, 4 µl of 1 µM in vitro phosphorylated (except where noted) single-stranded siRNA, duplexed siRNA or single-stranded DNA were added to the mix and incubated at 30 °C for 30 minutes. The final reaction was carried out in 20 µl which also contained 1mM ATP, 0.2 mM GTP, 8 units of RNAsin, 0.3 µg Creatine phosphokinase and 25 mM creatine phosphate. No-ATP reactions lacked ATP, GTP and the regeneration system. After a 2 hour incubation at 30 °C , RNAs were extracted using Trizol and chloroform and precipitated with isopropyl alcohol.

Example 4. Gene targeting and mice

Targeting construct was obtained by screening the lambda phage 3' HPRT library described in (Zheng et al., Nucleic Acids Res. 27, 2354 (1999)). The resultant targeting construct, containing exons 3-6 of mAgo2, was electroporated into mouse embryonic stem (ES) cells. Targeted clones were injected into C57BL/6 blastocysts to generate chimeras, which were crossed with C57BL/6 mice. Mouse genotyping was performed by Southern blot after digestion of genomic DNA with HindIII. The probe was amplified from genomic DNA using primer sequences 5'GACAATAGTGCAGAGACTTGC3' and 5'GGGCAGCCTGAGAATTGA3'. GenBank Accession Number for mouse Ago2 is AB081472. The Ago2 gene trap cell line RRE192 was obtained from Bay Genomics(Stryke et al., Nucleic Acids Res. 31, 278 (2003)).

Example 5. In situ hybridization

In situ hybridization was performed on whole-mount embryos essentially as described (Belo et al., Mech Dev. 68, 45 (1997)). Riboprobes for in situ hybridization were synthesized from T7-promoter containing PCR products corresponding to the 3' UTRs of Ago2 or Ago3. The Ago2 probe was amplified from genomic DNA using the primers 5'AGCTGTGAAGGCTCTGAG3' and 5'CAGTCCTACAGGACAAATCT3', and the Ago3 probe was similarly constructed using primers, AGGCTGTACAGATTCACCAAGATA and CCTTTACAAGAATAGATGCACATT.

Example 6. MEF Culture, transfection, and gene silencing assays

Day 10.5 embryos were dissected and diced in trypsin. Mouse embryo fibroblasts (MEFs) were cultured in DMEM + 10% FBS. MEFs were transfected in 24 well plates using Lipofectamine reagent according to the manufacturer's recommendations. Where indicated, each well received 2.5 picomoles of siRNA and 1ug of plasmid DNA. Dual luciferase assays (Promega) were carried out by cotransfecting cells with plasmids containing firefly luciferase under the control of the SV40 promoter (pGL3-Control, Promega) and Renilla luciferase under the control of the SV40 early enhancer/promoter region (pSV40, Promega). Luciferase siRNA was obtained from Dharmacon (siStarter, anti-luc siRNA-1). GFP (pEGFP-C1) and dsRed (pDsRed-express-N1) plasmids were obtained from Clontech. EGFP siRNA was obtained from Dharmacon (EGFP duplex). Ago1 and Ago2 expression plasmids were as described for the IP experiments, except that proteins were fused to an HA tag rather than a myc tag. Constructs for the translational repression assay were kindly provided by P. Sharp (Doench et al., Genes Dev. 17, 438 (2003)).

Example 7. RT-PCRs

RNA was extracted from cells and embryos using Trizol Reagent. Reverse transcription was conducted using Superscript-II RT from Invitrogen according to manufacturer's instructions. Subsequent PCR reactions were carried out using the following primers (5'-3'): mAgo1, GCATTTCAAGCAGAAATATAACCTTCA

and AGACTTTGATCTCAATCCC
ATTGTAG. MAgo2, GTACTTCAAGGACAGGCACAAGCTG and
TGGCAATTGC
TTTGTTCCTGC. MAgo3, GCTGCAGCTGAAGTACCCACA and
GTACTGGAGCATA
GGTGCTGGAAGTA. Mouse β-actin, CACTATTGGCAACGAGCGGT and
CTTCATGGT
GCTAGGAGCCA.

Example 8. MiRNA microarrays

RNA was recovered from immunoprecipitates with Trizol (Invitrogen) and conjugated with a Cy3 dinucleotide using T4 RNA ligase (NEB). Labeled RNA was hybridized to microarrays containing probes to 152 human mature microRNA sequences, washed, and scanned on a Genepix 400B array scanner. Log-ratios of Cy3/Cy5 values were global median center normalized for Ago-1, Ago-2, Ago-3 immunoprecipitates. For the control immunoprecipitate, data was normalized by a constant that was the average of the normalization constant for the Ago-1, Ago-2, Ago-3 datasets. Data was sorted in descending order for the Ago-2 dataset and a heat map generated using Treeview (Stanford University).

Example 9. miRNA Microarray Results.

Ago1-, Ago2- and Ago3-associated RNAs were hybridized to microarrays that report the expression status of 152 human microRNAs. Patterns of associated RNAs were identical within experimental error in each case (Fig. 9, Panel A). Additionally, each of the tagged Ago proteins associated similarly with a co-transfected siRNA (Fig. 9, Panel C). Previous studies have used tagged siRNAs to affinity purify Argonaute-containing RISC (Martinez et al., *supra*). These preparations, containing mixtures of at least two mammalian Argonautes, were capable of cleaving synthetic mRNAs that were complementary to the tagged siRNA. The ability of purified complexes containing individual Argonaute proteins to catalyze similar cleavages was examined. Surprisingly, irrespective of the siRNA sequence, only Ago2-containing RISC was able to catalyze cleavage (Fig. 9, Panel

B; Fig. 14). All three Ago proteins were similarly expressed and bound similar amounts of transfected siRNA (Fig. 1 Panels C and D).

These results demonstrated that mammalian Argonaute complexes are biochemically distinct, with only a single family member being competent for mRNA cleavage. To examine the possibility that Ago proteins might also be biologically specialized, the mouse Ago2 gene were disrupted by targeted insertional mutagenesis (Fig. 15; Fig. 10, Panel A) (Zheng et al., *supra*). Intercrosses of Ago2 heterozygous produced only wild-type and heterozygous offspring, strongly suggesting that disruption of Ago2 produced an embryonic-lethal phenotype. Ago2 deficient mice display several developmental abnormalities beginning approximately halfway through gestation. Both gene-trap and in situ hybridization data of day 9.5 embryos show broad expression of Ago2 in the embryo, with some hotspots of expression in the forebrain, heart, limb buds and branchial arches (Fig 10, Panels F and G). The most prominent phenotype is a defect in neural tube closure (Fig. 10, Panels D and E), often accompanied by apparent mispatterning of anterior structures including the forebrain (Fig. 10, Panels C and D). Roughly half of the embryos display complete failure of neural tube closure in the head region (Fig. 10, Panel E), while all embryos display a wavy neural tube in more caudal regions. Mutant embryos also suffer from apparent cardiac failure. The hearts are enlarged, and often accompanied by pronounced swelling of the pericardial cavity (Fig. 10, Panel C). By day 10.5, mutant embryos are severely developmentally delayed compared to wildtype and heterozygous littermates (Fig. 10, Panel B). This large difference in size, like the apparent cardiac failure, may be accounted for by a general nutritional deficiency caused by yolk sac and placental defects (Conway et al., Genesis 35, 1 (2003)), as histological analysis reveals abnormalities in these tissues.

Not all Argonaute proteins are required for successful mammalian development (Deng et al., Cell 2, 819, (2002); Kuramochi-Miyagawa et al., Development 131, 839 (2004)). Ago subfamily members are expressed in overlapping patterns in humans (Sasaki et al., Genomics 82, 323 (2003)). In situ hybridization demonstrates overlapping expression patterns for Ago2 and Ago3 in mouse embryos (Fig 10, Panel F; Fig. 16). Considered together with the essentially

identical patterns of miRNA binding, the results suggest the possibility that the ability of Ago2 to assemble into catalytically active complexes might be critical for mouse development. Although most miRNAs regulate gene expression at the level of protein synthesis, recently miR196 has been demonstrated to cleave the mRNA encoding HoxB8, a developmental regulator (Yekta et al., Science 304, 594 (2004)). Evolutionary conservation of an essential cleavage-competent RISC in organisms in which miRNAs predominantly act by translational regulation raises the possibility that target cleavage by mammalian miRNAs might be more important and widespread than previously appreciated.

Numerous studies have indicated that experimentally triggered RNAi in mammalian cells proceeds through siRNA-directed mRNA cleavage since in many, but not all, cases reiterated binding sites are necessary for repression at the level of protein synthesis (see for example (Bartel, Cell 116, 281 (2004); Doench et al., *supra*; Kiriakidou et al., Genes Dev. 18, 1165 (2004)). If Ago2 were uniquely capable of assembling into cleavage competent complexes in mice, then embryos or cells lacking Ago2 might be resistant to experimental RNAi. To address this question, mouse embryo fibroblasts (MEF) were prepared from E10.5 embryos from Ago2 heterozygous intercrosses. RT-PCR analysis and genotyping revealed that wild-type, mutant and heterozygous MEF populations were obtained. Importantly, MEF also express other Ago proteins, including Ago1 and Ago3 (Fig. 11, Panel A). Ago2 null MEF were unable to repress gene expression in response to an siRNA (Fig. 11, Panel B; Fig. 17). This defect could be rescued by addition of a third plasmid that encoded human Ago2 but not by Ago1 (Fig. 11, Panel B). In contrast, responses were intact for a reporter of repression at the level of protein synthesis, mediated by an siRNA binding to multiple mismatched sites (Doench et al., *supra*) (Fig. 11, Panel C).

Example 10. Mapping of determinants for cleavage

Since Ago2 was unique in its ability form cleavage-competent complexes, determinants of this capacity were mapped. Deletion analysis indicated that an intact Ago2 was required for RISC activity (Fig. 18). Therefore, the sequence of highly conserved but cleavage-incompetent Ago proteins was used as a guide to the

construction of Ago2 mutants. A series of point mutations included H634P, H634A, Q633R, Q633A, H682Y, L140W, F704Y and T744Y. While all of these mutations retain siRNA binding activity and most retain cleavage activity, changes at Q633 and H634 have a profound effect on target cleavage (Fig. 12). Both the Q633R and H634P mutations, in which residues were changed to corresponding residues in Ago1/3, abolished catalysis. Changing H634 to A also inactivated Ago2, while a similar change, Q633A, was permissive for cleavage. Thus, even relatively conservative changes can negate the ability of Ago2 to form cleavage-competent RISC.

Several possibilities could explain a lack of cleavage activity for Ago2 mutants. Such mutations could interfere with the proper folding of Ago2. However, this seems unlikely as those same residues presumably permit proper folding in closely related Argonaute proteins, and mutant Ago2 proteins retained the ability to interact with siRNAs. Alternatively, cleavage-incompetent Ago2 mutants could lose the ability to interact with the putative Slicer. Finally, Ago2 itself might be Slicer, with the conservative substitutions altering the active center of the enzyme in a way that prevents cleavage. The last possibility predicted that an active enzyme with relatively pure Ago2 protein may be reconstituted. Ago2 was immunoaffinity purified from 293T cells and attempted to reconstitute RISC in vitro. Incubation with the double-stranded siRNA produced no significant activity, whereas Ago2 could be successfully programmed with single-stranded siRNAs to cleave a complementary substrate (Fig. 13, Panel A). Formation of the active enzyme was unaffected by first washing the immunoprecipitates with up to 2.5M NaCl or 1M urea. A 21nt single stranded DNA was unable to direct cleavage (Fig. 13, Panel A). Programming could be accomplished with different siRNAs that direct activity against different substrates (Fig. 19). RISC is formed though a concerted assembly process in which the RISC-Loading Complex (RLC) acts in an ATP-dependent manner to place one strand of the small RNA into RISC (Nykanen et al., Cell 107, 309 (2001); Pham et al., Cell 117, 83 (2004); Tomari et al., Cell 116, 831 (2004)). In vitro reconstitution occurs in the absence of ATP, suggesting that Ago2 could be programmed with siRNAs without a need for the normal assembly process (Fig. 13, Panel A). However, in vitro reconstitution of RISC still required the essential

characteristics of an siRNA. For example, single-stranded siRNAs that lack a 5' phosphate group cannot reconstitute an active enzyme.

While consistent with the possibility that the catalytic activity of RISC is carried within Ago2, these results do not rule out the possibility that a putative Slicer co-purifies with Ago2. To demonstrate more conclusively that Ago2 is Slicer, the crystal structure of an Argonaute protein from an archebacterium, *Pyrococcus furiosus*, was analyzed. This structure revealed that the PIWI domain folds into a structure analogous to the catalytic domain of RNAseH and ASV integrase. The notion that such a domain would lie at the center of RISC cleavage is consistent with previous observations. RNAseH and integrases cleave their substrates leaving 5' phosphate and 3' hydroxyl groups through a metal catalyzed cleavage reaction (Chapados et al., J. Mol. Biol. 307, 541 (2001); Yang et al., Strcuture 3, 131 (1995)). Notably, previous studies have strongly indicated that the scissile phosphate in the targeted mRNA is cleaved via a metal ion in RISC to give the same phosphate polarity (Schwarz et al., Curr. Biol. 14, 787 (2004)). The in vitro data are consistent with the reconstituted RISC also requiring a divalent metal (Fig. 20). The active center of RNAseH and its relatives consists of a catalytic triad of three carboxylate groups contributed by aspartic or glutamic acid (Chapados et al., *supra*; Yang et al., *supra*). These coordinate the essential metal and activate water molecules for nucleolytic attack. Reference to the known structure of RNAseH reveals two aspartate residues in the archeal Ago protein present at the precise spatial locations predicted for formation of an RNAseH-like active site. These align with identical residues in the human Ago2 protein (Fig. 21). Therefore, to test whether the PIWI domain of Ago2 provides catalytic activity to RISC, the two conserved aspartates, D597 and D669, were changed to alanine, with the prediction that either mutation would inactivate RISC cleavage. Consistent with this hypothesis, the mutant Ago2 proteins were incapable of assembling into a cleavage-competent RISC in vitro or in vivo, despite retaining the ability to bind siRNAs (Fig. 13, Panels B-D).

Considered together, the data provide strong support for the notion that Argonaute proteins are the catalytic components of RISC. Firstly, the ability to form an active enzyme is restricted to a single mammalian family member, Ago2. This

conclusion is supported both by biochemical analysis and by genetic studies in mutant MEF. Secondly, single amino acid substitutions within Ago2 that convert residues to those present in closely related proteins negate RISC cleavage. Thirdly, the structure of the P. furiosis Argonaute protein reveals provocative structural similarities between the PIWI domain and RNAseH domains, providing a hypothesis for the method by which Argonaute cleaves its substrates. This hypothesis was tested by introducing mutations in the predicted Ago2 active site.

Example 11. Protein expression and purification

The full length Argonaute gene from *Pyroccocus furiosus* (PfAgo) was cloned into a pSMT3 vector. PfAgo was expressed as an Smt3 fusion with an N-terminal histidine tag in BL21-RIPL cells. Smt3_Argonaute protein was purified with an NTA-agarose affinity column, and Smt3 was removed using Ulp1 protease, which cuts right after Smt3. The pSMT3 vector-Ulp1 protease system was a generous gift from Dr. Chris Lima. PfAgo was further purified with a heating step, as this protein is from a hyperthermophilic organism, anion exchange chromatography and gel filtration. Purified protein was concentrated to 12.5 mg/ml in 50mM Tris-HCl (pH8.0) and 300 mM NaCl. Se-Met substituted protein was expressed using metabolic inhibition of methionine biosynthesis as described in (G.D. Van Duyne, R.F. Standaert, P.A. Karplus, S.L. Schreiber, J. Clardy, J Mol Biol 229, 105-24 (1993)). Se-Met incorporation was confirmed by mass spectrometry.

Example 12. Crystallization and data collection

Initial crystals were grown by vapor diffusion using the hanging-drop method in the presence of organic solvents. The quality of crystals was significantly improved by several rounds of microseeding. Selenomethionine (Se-Met) substituted protein crystals were obtained by microseeding with native crystals. Mercury-derivatized crystals were prepared by soaking native crystals in 1mM p-chloromercuriphenylsulfonic acid for 5 hours. For cryoprotection crystals were soaked for 1 min in crystallization solution containing increasing amounts of ethylenglycol (EG) in 5% steps to a final EG concentration of 40%(v/v). Crystals

diffracted to approximately 2 Å resolution. All data were collected to a resolution of 2.25Å under cryogenic conditions (100K) at beamline X25 at the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory. Data were processed with HKL2000 (http://www.hkl-xray.com) (Table 1 provided in Figure 23).

Crystallization condition for native crystal:

1) Well solution as Water; and 2) Mixing 2 µl of 12.5 mg/ml PfAgo protein with 1 µl of water and 0.3 ul of 7% 1-butanol

Crystallization condition for Se-crystal:

1) Well solution as Water; and 2) Mixing 2 µl of 12.5 mg/ml PfAgo protein with 0.3 µl of 7% 1-butanol.

Example 13. Structure determination

Phases were calculated from a three-wavelength anomalous dispersion (MAD) experiment at the selenium inflection, peak and high remote energies using a Se-Met substituted crystal at the peak energy for the mercury derivative. 17 selenium sites were located using SnB (C.M. Weeks, R. Miller, J. of Applied Crystallography 32, 120-124 (1999)) and a single Hg site was located by calculating an anomalous difference Fourier map using initial phases calculated from the selenium data. Data from all three wavelengths for the Se-Met derivative and one wavelength for the Hg derivative were used for heavy atom site refinement by the program SHARP (E. delaFortelle, G. Bricogne, Meth. Enzymol. 276, 472-494 (1997)), followed by solvent flattening. A partial model was built using the program wARP (A. Perrakis, R. Morris, V.S. Lamzin, Nature Structure Biol. 6, 458-463 (1999)). The program SIGMAA (C.C.C.P.N.4. (Acta Crystallogr. D50, 760, Daresbury, UK, 1994)) was used to combine the partial structure model with the experimental phases. Iterative model building using the program O (T.A. Jones, M. Kjeldgaard, Methods Enzymol. 277, 173-208 (1997)) and crystallographic refinement with the program CNS (A.T. Brünger et al., Acta Crystallogr. D54, 905-921 (1998)) lead to the final model that contains 5913 protein atoms, and 77 water

molecules (Table 1 provided in Figure 23). Several loops are disordered in the structure and were not included: L26-G38, I253-K256, E278-V281, L347-L354, and S414-K442.

Example 14. UV crosslinking

PfAgo or GST were incubated with a 21-mer 5'-32 P-labeled ssRNA with an IodoU at the 5' end and unlabeled competitor ssRNA for 30 min at 30 °C. Incubation was carried out in 10 mM Tris-HCl (pH 7.5), 2 mM $MgCl_2$, and 150 mM KCl. UV crosslinking was done using a Stratalinker (Stratagene) at 312 nm for 20 min at room temperature. Double-stranded RNA probes were gel purified after annealing the 5'- ^{32}P-labeled ssRNA with an unlabeled complementary strand to form a ds-siRNA (including a 2-nucleotide 3'overhang and a 5'-phosphate group).

CLAIMS

1. A crystalline Argonaute.

2. A method of determining the three-dimensional structure of an Argonaute protein or a mutant, derivative, variant, analogue, homologue, sub-domain or fragment thereof comprising:

(a) aligning the amino acid sequence of the Argonaute mutant, derivative, variant, analogue, homologue, sub-domain or fragment with the amino acid sequence set forth in SEQ ID NO: 5 to match homologous regions of the amino acid sequences;

(b) modelling the structure of the matched homologous regions of said target Argonaute protein of unknown structure on the corresponding regions of the Argonaute protein structure as defined by the atomic co-ordinates as set forth in Table 3; and

(c) determining a conformation for the Argonaute mutant, derivative, variant, analogue, homologue, sub-domain or fragment which substantially preserves the structure of said matched homologous regions.

3. A method of identifying an agent that binds an Argonaute protein comprising:

(a) applying a 3-dimensional molecular modeling algorithm to the atomic coordinates of an Argonaute protein shown in Table 3 to determine the spatial coordinates of the binding pocket of the Argonaute protein; and

(b) electronically screening the stored spatial coordinates of a set of candidate agents against the spatial coordinates of the Argonaute protein binding pocket to identify agents that can bind to the Argonaute protein.

4. A computer-based method for the analysis of the interaction of a molecular structure with an Argonaute protein, comprising:

(a) providing a structure comprising a three-dimensional representation of said Argonaute protein or a portion thereof, which representation comprises all or a portion of the coordinates set forth in Table 3;

(b) providing a molecular structure to be fitted to said Argonaute protein structure; and

(c) fitting the molecular structure to the Argonaute protein structure of (a).

5. A computer-readable storage medium encoded with the atomic coordinates or an Argonaute protein as shown in Table 3.

6. A data array comprising the atomic coordinates of an Argonaute protein as set forth in Table 3.

7. An electronic representation of a crystal structure of an Argonaute protein.

8. An electronic representation of a binding site of the Argonaute protein.

9. An electronic representation of a domain of the Argonaute protein.

10. An electronic representation of an agent in a binding site of an Argonaute protein.

11. A method for obtaining a crystal of an Argonaute protein, comprising subjecting an Argonaute protein at 10-15 mg/ml to crystallization conditions for a time sufficient for crystal formation.

12. A method of identifying an agent that modulates the activity of an RNAi construct, comprising identifying an agent that modulates the expression and/or activity of an Argonaute protein.

13. A method of identifying an agent that potentiates the activity of an RNAi construct, comprising identifying an agent that increases the expression and/or activity of an Argonaute protein.

14. A method of identifying an agent that modulates the activity of an RNAi construct comprising:

(a) providing an isolated or recombinant Argonaute protein; and

(b) assaying the activity of said Argonaute protein in the presence of a candidate agent,

wherein a change in the activity of said Argonaute protein in the presence of a candidate agent is indicative of said candidate agent capable of modulating the activity of an RNAi construct.

15. A composition for targeted gene inhibition comprising an agent that modulates the RNase activity of an Argonaute protein.

16. A pharmaceutical composition comprising the composition of claim 15 and a physiologically acceptable carrier.

17. A cell line that overexpresses an Argonaute protein.

18. An assay for identifying nucleic acid sequences for conferring a particular phenotype in a cell, comprising:

(a) constructing a library of nucleic acid sequences oriented to produce double stranded RNA;

(b) introducing a dsRNA library into a culture of target cell line of claim 17;

(c) identifying members of the library which confer a particular phenotype on the cell, and identifying the sequence from the cell which is identical or homologous to the library member.

19. A nucleic acid composition comprising:

(a) a first nucleic acid comprising an RNAi construct and

(b) a second nucleic acid encoding an Argonaute protein.

20. The nucleic acid composition of claim 19, wherein the RNAi construct comprises a nucleotide sequence encoding a single-strand siRNA.

21. A pharmaceutical composition comprising the nucleic acid composition of claim 19 and a physiologically acceptable carrier.

22. A cell expressing the nucleic acid composition of claim 19.

Fig 1

Fig 2A

Fig 2B

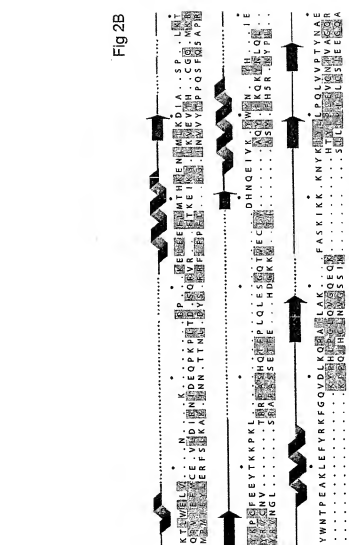


Fig 3A,B

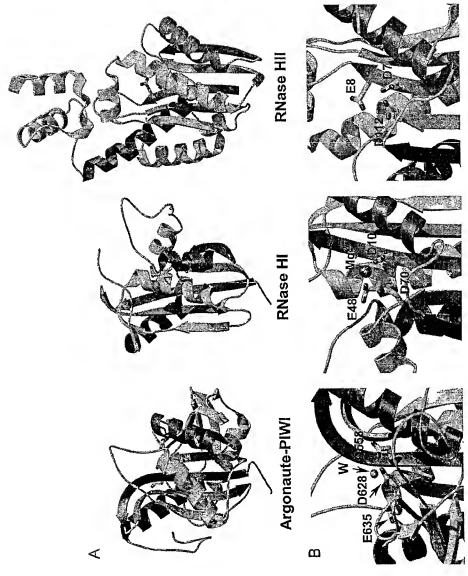

A
Argonaute-PIWI
RNase HI
RNase HII
B
W
D628
E635
E48
Mg
D10
D70
E8
D12
D7

Fig 3C

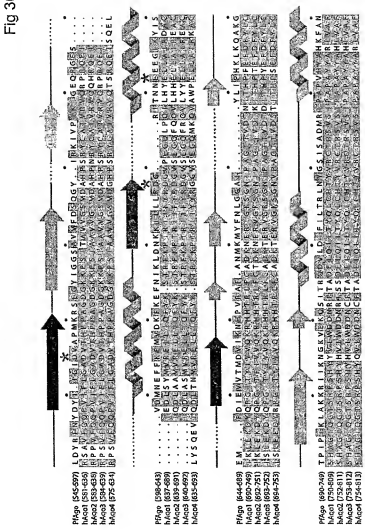
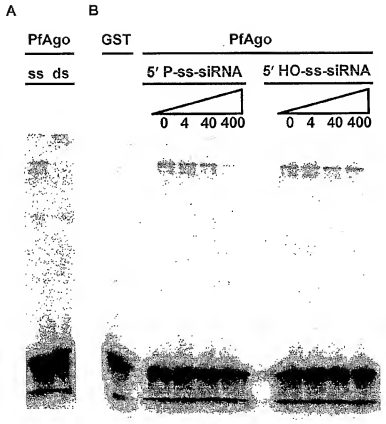


Fig 4


A
B
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ss ds
GST
PfAgo
5′ P-ss-siRNA
5′ HO-ss-siRNA
0 4 40 400
0 4 40 400

Fig 5A

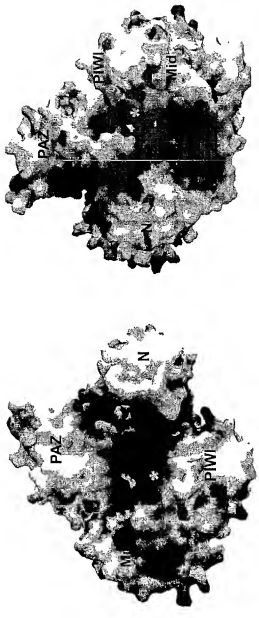


Fig 5B

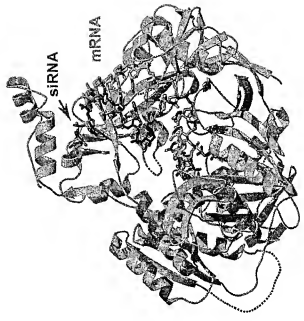
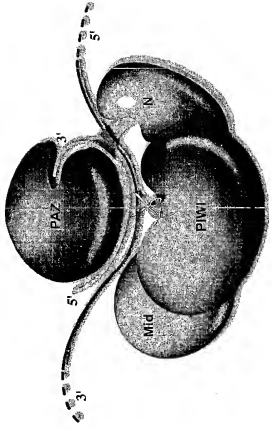


Fig 5C




PfAgo (152-188) MKTLWELV . . . N . . . K . . . . . DP . . KELEEFEMTHRENLMLKDIA . . SP . . LRT
hAgo1 (226-275) QPVLEFMCE VLDIRNIDEQPKPETD . SQAVR . . PTAEIKG . LKYEVTH . CGQ . MER
DmAgo2 (602-652) . MRMTFYLERFSLKAK . INN . TTHL . DYS . AMFLLPTEL . . RG . LNKVYTTPPQSFIQSAPR
PfAgo (189-219) VYYPCFEEYTKKPKL . . . . . DIHQEIYK . YWYN . YH . . . IE
hAgo1 (276-318) KYRVCNV . . . . . TRRKASHQTFPLQLESGQTVECTV . . . . . AQY . FKQKYNLCL . .
DmAgo2 (653-689) VYVLVNGL . . . . . SRAMASSFTEE . . . HDSKKV . . . . . AYIC . RHSR . NYPLV . .
PfAgo (210-273) RYWNTPEAKLEFYRKFGQVDLKQFAILAK . . . FASKIKK . KNYKLYLLPQLVVPTYNAE
hAgo1 (319-349) . . . . . KYPHLFCLQVTSQEQKK . . . . . HTVTPLLVCNLVAGQR
DmAgo2 (690-726) . . . . . KAPQLHCLHMYGSSIN . . . . . STILPTILCSHEDQA

Figure 6

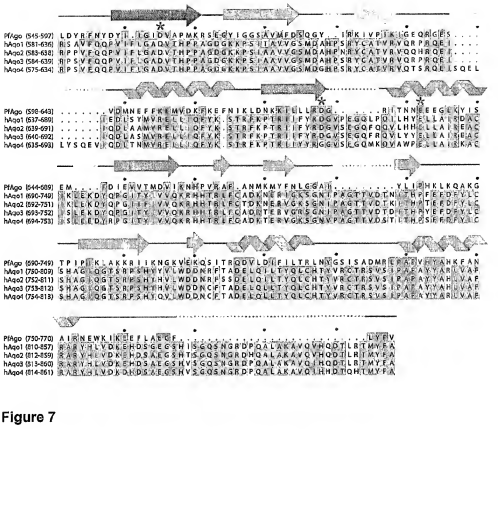


Figure 7

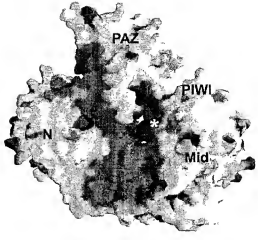


Figure 8

Figure 9

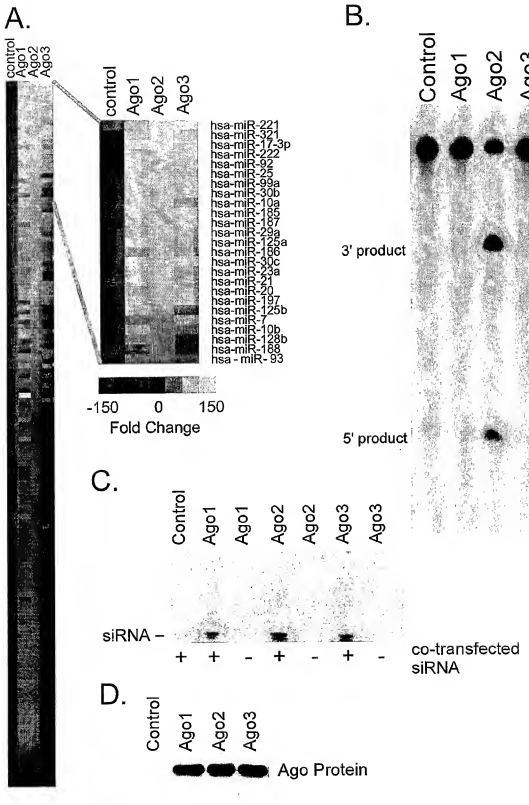

A.
control
Ago1
Ago2
Ago3
hsa-miR-221
hsa-miR-321
hsa-miR-17-3p
hsa-miR-222
hsa-miR-92
hsa-miR-25
hsa-miR-99a
hsa-miR-30b
hsa-miR-10a
hsa-miR-195
hsa-miR-16
hsa-miR-29a
hsa-miR-125a
hsa-miR-196
hsa-miR-30c
hsa-miR-23a
hsa-miR-21
hsa-miR-20
hsa-miR-197
hsa-miR-125b
hsa-miR-7
hsa-miR-10b
hsa-miR-128b
hsa-miR-188
hsa-miR-93
-150 0 150
Fold Change
B.
Control
Ago1
Ago2
Ago3
3' product
5' product
C.
Control
Ago1
Ago1
Ago2
Ago2
Ago3
Ago3
siRNA –
+ + - + - + -
co-transfected siRNA
D.
Control
Ago1
Ago2
Ago3
Ago Protein

Figure 10

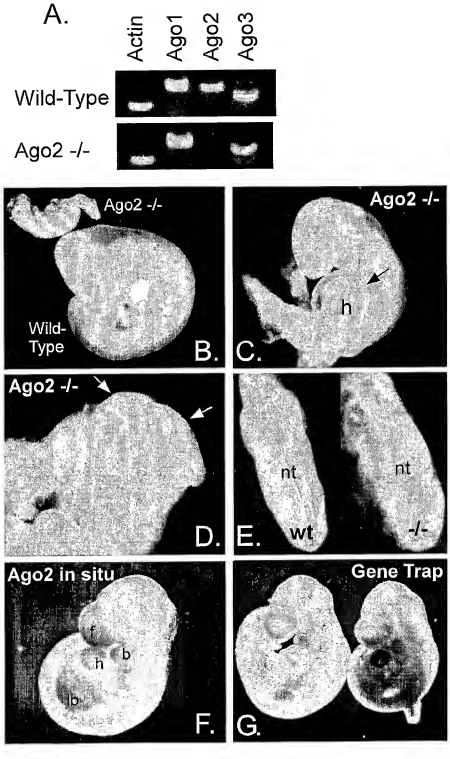
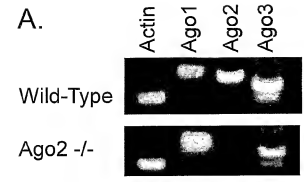
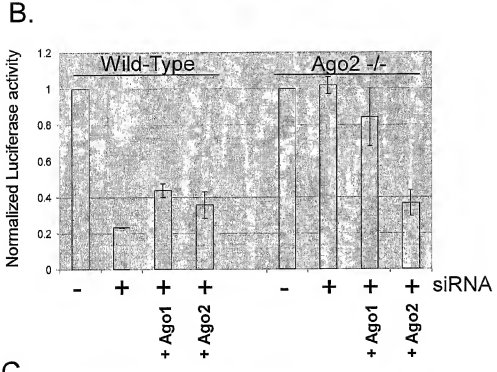

A.
Actin
Ago1
Ago2
Ago3
Wild-Type
Ago2 -/-
Ago2 -/-
Wild-Type
B.
Ago2 -/-
h
C.
Ago2 -/-
D.
nt
nt
wt
-/-
E.
Ago2 in situ
f
h
b
lb
F.
Gene Trap
G.

Figure 11


A.
Actin
Ago1
Ago2
Ago3
Wild-Type
Ago2 -/-


B.
Normalized Luciferase activity
Wild-Type
Ago2 -/-
siRNA
+ Ago1
+ Ago2

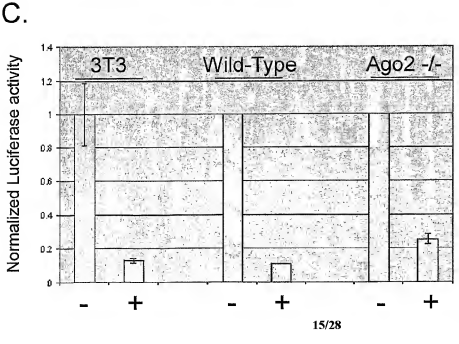
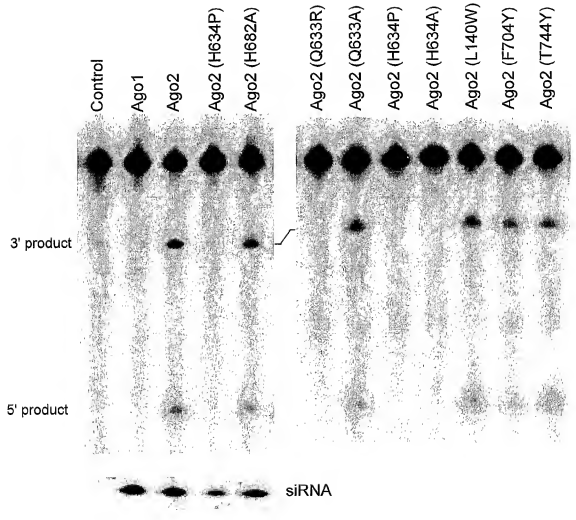

C.
Normalized Luciferase activity
3T3
Wild-Type
Ago2 -/-
mismatched siRNA

Figure 12


Control
Ago1
Ago2
Ago2 (H634P)
Ago2 (H682A)
Ago2 (Q633R)
Ago2 (Q633A)
Ago2 (H634P)
Ago2 (H634A)
Ago2 (L140W)
Ago2 (F704Y)
Ago2 (T744Y)
3' product
5' product
siRNA

A.
Reconstitute Ago2 with :
no siRNA
ss siRNA
ds siRNA
ss siRNA
ss siRNA, no 5'P
ss siRNA, no ATP
ss siRNA
ss DNA
3' product
5' product
Ago2
HSP90
heavy chain
light chain
Protein Gel
B.
Control
Ago2(WT)
Ago2(D597A)
Ago2(D669A)
Ago2 (WT)
Ago2(D597A)
Ago2(D669A)
siRNA co-transfection
in vitro reconstitution
C.
Control
Ago2(WT)
Ago2(D597A)
Ago2(D669A)
Ago2
D.
Control
Ago2(WT)
Ago2(D597A)
Ago2(D669A)
siRNA

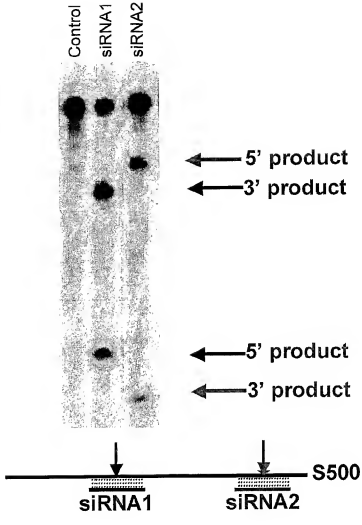
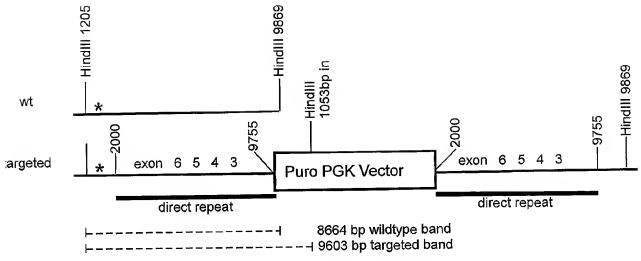

Control
siRNA1
siRNA2
5' product
3' product
5' product
3' product
S500
siRNA1
siRNA2

Figure 14


HindIII 1205
HindIII 9869
HindIII 1053bp in
wt
targeted
2000
9755
exon 6 5 4 3
Puro PGK Vector
2000
9755
exon 6 5 4 3
HindIII 9869
direct repeat
direct repeat
8664 bp wildtype band
9603 bp targeted band

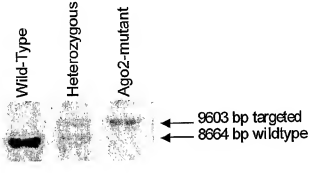

Wild-Type
Heterozygous
Ago2-mutant
9603 bp targeted
8664 bp wildtype

Figure 15

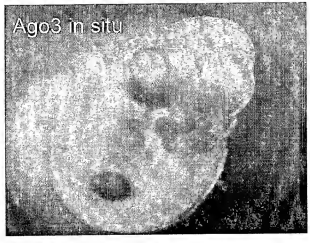


Figure 16

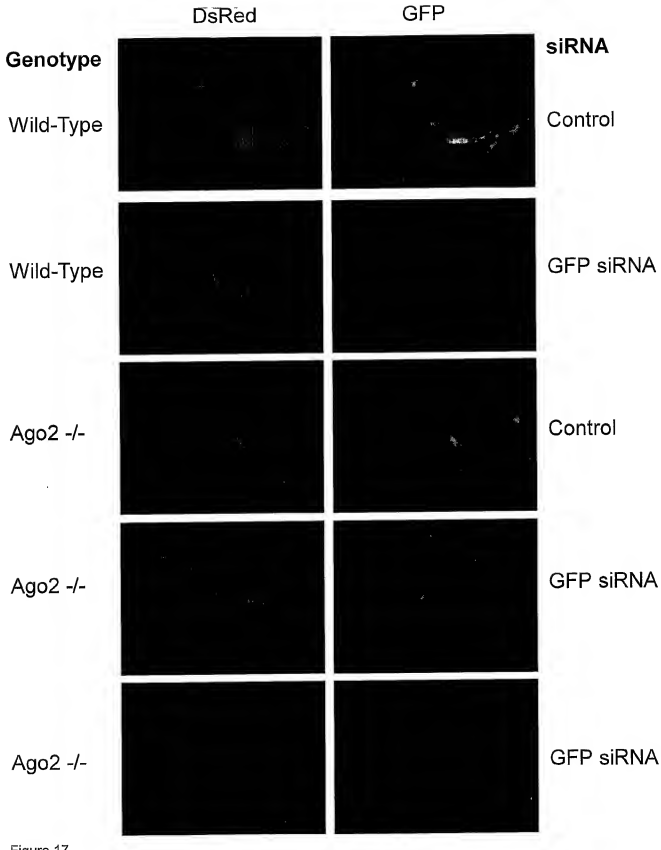

DsRed
GFP
Genotype
siRNA
Wild-Type
Control
Wild-Type
GFP siRNA
Ago2 -/-
Control
Ago2 -/-
GFP siRNA
Ago2 -/-
GFP siRNA

Figure 17

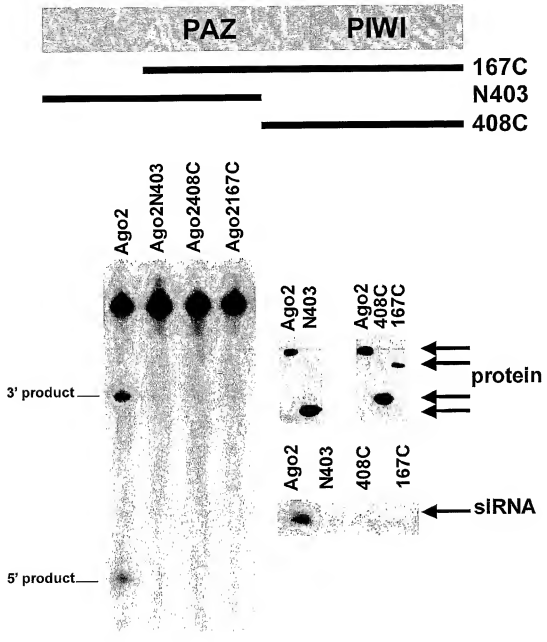

PAZ
PIWI
167C
N403
408C
Ago2
Ago2N403
Ago2408C
Ago2167C
Ago2 N403
Ago2 408C 167C
protein
3' product
Ago2 N403 408C 167C
siRNA
5' product

Figure 18

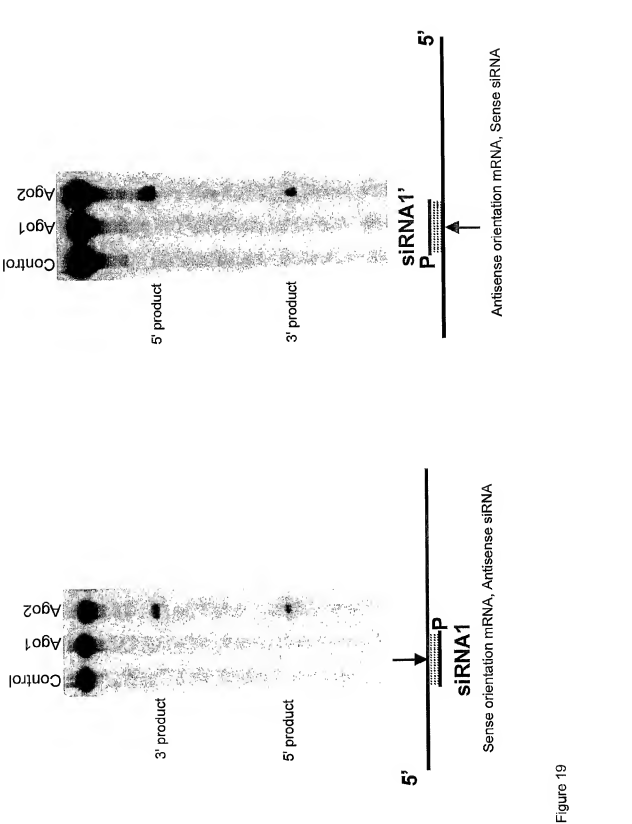

Control
Ago1
Ago2
3' product
5' product
5'
P
siRNA1
Sense orientation mRNA, Antisense siRNA
Control
Ago1
Ago2
5' product
3' product
siRNA1'
P
5'
Antisense orientation mRNA, Sense siRNA

Figure 19

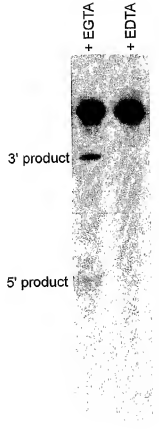


Figure 20

```
                             595                                          634
Human Ago2                   GADVTHPPAGDGKKPSIAAVVGSMD-AHPNRYCATVRVQQHRQKIIQDLA-------------AMVRELLIQFYK-STR-
Mouse Ago2                   GADVTHPPAGDGKKPSIAAVVGSMD-AHPNRYCATVRVQQHRQEIIQDLA-------------AMVRELLIQFYK-STR-
Rat                          GADVTHPPAGDGKKPSIAAVVGSMD-AHPNRYCATVRVQQHRQEIIQDLA-------------AMVRELLIQFYK-STR-
Bos taurus                   GADVTHPPAGDGKKPSIAAVVGSMD-AHPNRYCATVRVQQHRQEIIQDLA-------------AMVRELLIQFYK-STR-
Rabbit                       GADVTHPPAGDGKKPSIAAVVGSMD-AHPNRYCATVRVQQHRQEIIQDLA-------------AMVRELLIQFYK-STR-
Drosophila Ago1              GADVTHPPAGDNKKPSIAAVVGSMD-AHPSRYAATVRVQQHRQEIIQELS-------------SMVRELLIMFYK-STGG
Anopheles gambiae            GADVTHPPAGDNKKPSIAAVVGSMD-AHPSRYAATVRVQQHRQEIIQELS-------------SMVRELLIMFYK-STGG
Caenorhabditis briggsae      GCDITHPPAGDSRKPSIAAVVGSMD-AHPSRYAATVRVQQHRQEIISDLT-------------YMVRELLVQFYR-NTR-
C. elegans ALG-1             GCDITHPPAGDSRKPSIAAVVGSMD-AHPSRYAATVRVQQHRQEIISDLT-------------YMVRELLVQFYR-NTR-
C. elegans ALG-2             GCDITHPAAGDTRKPSIAAVVGSMD-AHPSRYAATVRVQQHRQEIITDLT-------------YMVRELLVQFYR-NTR-
Oryza sativa 1               GADVTHPHPGEDSSPSIAAVVASQDWPEVTKYAGLVSAQAHRQELIQDLFKVWQDPHRGTVTGGMIKELLISFKR-ATG-
Oryza sativa 2               GADVTHPHPGEDSSPSIAAVVASQDWPEVTKYAGLVSAQAHRQELIEDLYKIWQDPQRGTVSGGMIRELLISFKR-STG-
Arabidopsis Ago1             GADVTHPHPGEDSSPSIAAVVASQDWPEITKYAGLVCAQAHRQELIQDLFKEWKDPQKGVVTGGMIKELLIAFRR-STG-
Arabidopsis zwille           GADVTHPENGEESSPSIAAVVASQDWPEVTKYAGLVCAQAHRQELIQDLYKTWQDPVRGTVSGGMIRDLLISFRK-ATG-
Pyrococcus_furiosis          GIDVAPMKRSEGYIGGSAVMFDSQG-Y--IRKIVPIKIGEQRGES-VDMN-------------EFFKEMVDKFKEFNIK-
                              D                                            H

                                     669           683
Human Ago2                   FKPTRIIFYRDGVSEGQFQQVLHHELLAIR
Mouse Ago2                   FKPTRIIFYRDGVSEGQFQQVLHHELLAIR
Rat                          FKPTRIIFYRDGVSEGQFQQVLHHELLAIR
Bos taurus                   FKPTRIIFYRDGVSEGQFQQVLHHELLAIR
Rabbit                       FKPTRIIFYRDGVSEGQFQQVLHHELLAIR
Drosophila Ago1              YKPHRIILYRDGVSEGQFPHVLQHELTAIR
Anopheles gambiae            FKPHRIILYRDGVSEGQFPHVLQHELTAIR
Caenorhabditis briggsae      FKPARIVVYRDGVSEGQFFNVLQYELRAIR
C. elegans ALG-1             FKPARIVVYRDGVSEGQFFNVLQYELRAIR
C. elegans ALG-2             FKPARIVVYRDGVSEGQLFNVLQYELRAIR
Oryza sativa 1               QKPQRIIFYRDGVSEGQFYQVLLYELDAIR
Oryza sativa 2               EKPQRIIFYRDGVSEGQFYQVLLYELNAIR
Arabidopsis Ago1             HKPLRIIFYRDGVSEGQFYQVLLYELDAIR
Arabidopsis zwille           QKPLRIIFYRDGVSEGQFYQVLLYELDAIR
Pyrococcus_furiosis          LDNKKILLLRDG-------RITNNEEEGLK
                                        D
```

Figure 21

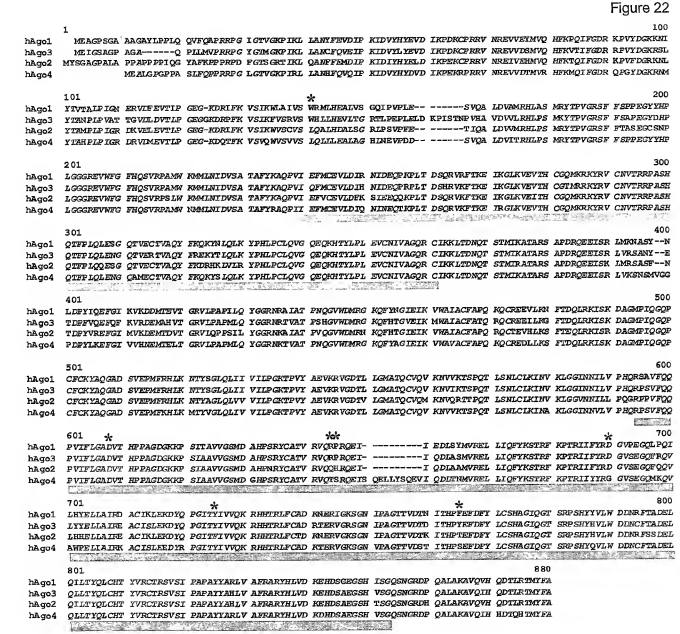

hAgo1
hAgo3
hAgo2
hAgo4

Figure 23

Table 1. Crystallographic Statistics

Space group	$P2_1$
Unit cell	a=69.72, b=104.19, c=74.01, α=90, β=102.83, γ=90

A. Data Reduction Statistics

	λ(Å)	Resolution(Å)	Measured Reflections	Unique Reflections	Percent Complete	I/σ(I)	R_{sym}[a]
Se peak	0.9791	2.25(2.33-2.25)	350855	48108(4820)	98.7(100)	42.6(6.03)	0.078(0.473)
Se edge	0.9796	2.25(2.33-2.25)	351677	48228(4852)	98.7(100)	41.8(5.50)	0.060(0.511)
Se remote	0.9638	2.25(2.33-2.25)	354296	48470(4848)	99.3(100)	41.6(4.34)	0.066(0.632)
Hg peak	1.0076	2.25(2.33-2.25)	354357	48293(4781)	99.8(100)	39.4(4.24)	0.086(0.666)

B. Phasing Statistics

	Acentric Phasing Power[b]		Centric Phasing Power	
	50-2.25Å	2.31-2.25Å	50-2.25Å	2.31-2.25Å
Se peak anomalous	2.912	0.616		
Se edge isomorphous	0.903	0.294	0.690	0.212
Se edge anomalous	1.234	0.287		
Se remote isomorphous	0.598	0.191	0.458	0.313
Se remote anomalous	1.389	0.313		
Hg peak isomorphous	0.801	0.406	0.717	0.331
Hg peak anomalous	0.301	0.069		

FOM[c]	50-2.25 Å	2.31-2.25 Å
Acentric reflections	0.553	0.305
Centric reflections	0.305	0.177

C. Refinement Statistics

Reflection used	500-2.25 Å
Number of atoms	5990(protein:5913, water:77)
R_{work}/free	0.2420/46298
R_{free}/free	0.2708/2528

D. Geometry

	Core	Allowed
Ramachandran plot(%)	84.2	15.8

Bond length RMSD(Å)	0.0066
Bond angle RMSD( )	1.273

[a] R_{sym};$R_{sym} = \sum|I-\langle I\rangle|/\sum\langle I\rangle$, calculated by retaining anomalous-mates and symmetry-mates as independent observations, respectively.
[b] Phasing power calculated as F_H/(calc)phase integrated lack of closure.
[c] FOM is weighted over F amplitude and phase as calculated by the program SHARP.

Figure 24

Table 2. Crystallographic Statistics

Space group	$P2_1$
Unit cell	a=69.72, b=104.19, c=74.01, α=90, β=102.83, γ=90

A. Data Reduction Statistics

	λ(Å)	Resolution(Å)	Measured Reflections	Unique Reflections	Percent Complete	I/σ(I)
Se peak	0.9791	2.25(2.33-2.25)	350855	48108(4820)	98.7(100)	42.6(6.03)
Se edge	0.9796	2.25(2.33-2.25)	351677	48228(4852)	98.7(100)	41.8(5.50)
Se remote	0.9638	2.25(2.33-2.25)	354296	48470(4848)	99.3(100)	41.5(4.34)
Hg peak	1.0076	2.25(2.33-2.25)	354357	48293(4781)	99.8(100)	38.4(4.24)

B. Phasing Statistics

	Acentric Phasing Power[b]		Centric Phasing Power	
	50-2.25Å	2.31-2.25Å	50-2.25Å	2.31-2.25Å
Se peak anomalous	2.912	0.616		
Se edge isomorphous	0.903	0.294	0.690	0.212
Se edge anomalous	1.234	0.267		
Se remote isomorphous	0.598	0.191	0.458	0.313
Se remote anomalous	1.389	0.313		
Hg peak isomorphous	0.801	0.406	0.717	0.331
Hg peak anomalous	0.301	0.069		

FOM[c]	50-2.25 Å	2.31-2.25 Å
Accentric reflections	0.553	0.305
Centric reflections	0.305	0.177

C. Refinement Statistics

Reflection used	38.14-2.25 Å
Number of atoms	6113(protein:5921, water:192)
R_{work}/#ref	0.228/46294
R_{free}/#ref	0.258/2528

D. Geometry

	Core	Allowed
Ramachandran plot(%)	85.6	14.4
Bond length RMSD(Å)	0.0064	
Bond angle RMSD( )	1.217	

[a] $R_{merge}/R_{sec} = \sum|I-<I>|/\sum(I)$, calculated by retaining anomalous-mates and symmetry-mates as independent observations, respectively.
[b] Phasing power calculated as F_H(calc)phase integrated lack of closure.
[c] FOM is weighted over F amplitude and phase as calculated by the program SHARP.

Table 3

```
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : CNS 1.1
REMARK   3   AUTHORS     : BRUNGER, ADAMS, CLORE, DELANO,
REMARK   3                 GROS, GROSSE-KUNSTLEVE, JIANG,
REMARK   3                 KUSZEWSKI, NILGES, PANNU, READ,
REMARK   3                 RICE, SIMONSON, WARREN
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 2.25
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) :  38.17
REMARK   3   DATA CUTOFF            (SIGMA(F)) : 0.0
REMARK   3   DATA CUTOFF HIGH         (ABS(F)) :  1695436.78
REMARK   3   DATA CUTOFF LOW          (ABS(F)) :    0.000000
REMARK   3   COMPLETENESS (WORKING+TEST)   (%) : 99.7
REMARK   3   NUMBER OF REFLECTIONS             : 48822
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD           : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION   : RANDOM
REMARK   3   R VALUE            (WORKING SET) : 0.227
REMARK   3   FREE R VALUE                      : 0.258
REMARK   3   FREE R VALUE TEST SET SIZE   (%) :  5.2
REMARK   3   FREE R VALUE TEST SET COUNT       :  2528
REMARK   3   ESTIMATED ERROR OF FREE R VALUE   : 0.005
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           :   6
REMARK   3   BIN RESOLUTION RANGE HIGH       (A) : 2.25
REMARK   3   BIN RESOLUTION RANGE LOW        (A) : 2.39
REMARK   3   BIN COMPLETENESS (WORKING+TEST) (%) :100.0
REMARK   3   REFLECTIONS IN BIN    (WORKING SET) :  7694
REMARK   3   BIN R VALUE           (WORKING SET) : 0.295
REMARK   3   BIN FREE R VALUE                    : 0.350
REMARK   3   BIN FREE R VALUE TEST SET SIZE  (%) :  5.2
REMARK   3   BIN FREE R VALUE TEST SET COUNT     :   422
REMARK   3   ESTIMATED ERROR OF BIN FREE R VALUE : 0.017
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS            : 5920
REMARK   3   NUCLEIC ACID ATOMS       :    0
REMARK   3   HETEROGEN ATOMS          :    0
REMARK   3   SOLVENT ATOMS            :  192
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : 39.1
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : 63.9
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) : -7.73
REMARK   3    B22 (A**2) :  1.12
REMARK   3    B33 (A**2) :  6.61
REMARK   3    B12 (A**2) :  0.00
REMARK   3    B13 (A**2) : -7.39
REMARK   3    B23 (A**2) :  0.00
```

```
REMARK   3
REMARK   3  BULK SOLVENT MODELING.
REMARK   3   METHOD USED : FLAT MODEL
REMARK   3   KSOL        : 0.327326
REMARK   3   BSOL        : 55.1711 (A**2)
REMARK   3
REMARK   3  ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM LUZZATI PLOT          (A) : 0.32
REMARK   3   ESD FROM SIGMAA                (A) : 0.27
REMARK   3   LOW RESOLUTION CUTOFF          (A) : 5.00
REMARK   3
REMARK   3  CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM C-V LUZZATI PLOT      (A) : 0.37
REMARK   3   ESD FROM C-V SIGMAA            (A) : 0.36
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3   BOND LENGTHS                   (A) : 0.007
REMARK   3   BOND ANGLES                (DEGREES) : 1.2
REMARK   3   DIHEDRAL ANGLES            (DEGREES) : 22.7
REMARK   3   IMPROPER ANGLES            (DEGREES) : 0.76
REMARK   3

REMARK   3  ISOTROPIC THERMAL MODEL : GROUP
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.      RMS    SIGMA
REMARK   3   MAIN-CHAIN BOND                (A**2) : NULL  ; NULL
REMARK   3   MAIN-CHAIN ANGLE               (A**2) : NULL  ; NULL
REMARK   3   SIDE-CHAIN BOND                (A**2) : NULL  ; NULL
REMARK   3   SIDE-CHAIN ANGLE               (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  NCS MODEL : NONE
REMARK   3
REMARK   3  NCS RESTRAINTS.                              RMS   SIGMA/WEIGHT
REMARK   3   GROUP  1  POSITIONAL              (A) : NULL  ; NULL
REMARK   3   GROUP  1  B-FACTOR            (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  PARAMETER FILE  1  : CNS_TOPPAR/protein_rep.param
REMARK   3  PARAMETER FILE  2  : CNS_TOPPAR/water_rep.param
REMARK   3  TOPOLOGY FILE   1  : CNS_TOPPAR/protein.top
REMARK   3  TOPOLOGY FILE   2  : CNS_TOPPAR/water.top
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: NULL
SEQRES   1 A  713  SER MSE LYS ALA ILE VAL VAL ILE ASN LEU VAL LYS ILE
SEQRES   2 A  713  ASN LYS LYS ILE ILE PRO ASP LYS ILE TYR VAL TYR ARG
SEQRES   3 A  713  LEU TYR SER ILE TYR ARG LEU ALA TYR GLU ASN VAL GLY
SEQRES   4 A  713  ILE VAL ILE ASP PRO GLU ASN LEU ILE ILE ALA THR THR
SEQRES   5 A  713  LYS GLU LEU GLU TYR GLU GLY GLU PHE ILE PRO GLU GLY
SEQRES   6 A  713  GLU ILE SER PHE SER GLU LEU ARG ASN ASP TYR GLN SER
SEQRES   7 A  713  LYS LEU VAL LEU ARG LEU LEU LYS GLU ASN GLY ILE GLY
SEQRES   8 A  713  GLU TYR GLU LEU SER LYS LEU LEU ARG LYS PHE ARG LYS
SEQRES   9 A  713  PRO LYS THR PHE GLY ASP TYR LYS VAL ILE PRO SER VAL
SEQRES  10 A  713  GLU MSE SER VAL ILE LYS HIS ASP GLU ASP PHE TYR LEU
SEQRES  11 A  713  VAL ILE HIS ILE ILE HIS GLN ILE GLN SER MSE LYS THR
SEQRES  12 A  713  LEU TRP GLU LEU VAL ASN LYS ASP PRO LYS GLU LEU GLU
SEQRES  13 A  713  GLU PHE LEU MSE THR HIS LYS GLU ASN LEU MSE LEU LYS
SEQRES  14 A  713  ASP ILE ALA SER PRO LEU LYS THR VAL TYR LYS PRO CYS
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FIGURE 25 CON'T
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SEQRES  15 A  713  PHE GLU GLU TYR THR LYS LYS PRO LYS LEU ASP HIS ASN
SEQRES  16 A  713  GLN GLU ILE VAL LYS TYR TRP TYR ASN TYR HIS ILE GLU
SEQRES  17 A  713  ARG TYR TRP ASN THR PRO GLU ALA LYS LEU GLU PHE TYR
SEQRES  18 A  713  ARG LYS PHE GLY GLN VAL ASP LEU LYS GLN PRO ALA ILE
SEQRES  19 A  713  LEU ALA LYS PHE ALA SER LYS ASN TYR LYS ILE TYR LEU
SEQRES  20 A  713  LEU PRO GLN LEU VAL VAL PRO THR TYR ASN ALA GLU GLN
SEQRES  21 A  713  LEU ALA LYS GLU ILE LEU GLU TYR THR LYS LEU MSE PRO
SEQRES  22 A  713  GLU GLU ARG LYS GLU LEU LEU GLU ASN ILE LEU ALA GLU
SEQRES  23 A  713  VAL ASP SER ASP ILE ILE ASP LYS SER LEU SER GLU ILE
SEQRES  24 A  713  GLU VAL GLU LYS ILE ALA GLN GLU LEU GLU ASN LYS ILE
SEQRES  25 A  713  ARG VAL ARG ASP ASP LYS GLY ASN SER VAL PRO ILE SER
SEQRES  26 A  713  GLN LEU LEU TRP THR ASN TYR SER ARG LYS TYR PRO VAL

SEQRES  27 A  713  ILE LEU PRO TYR GLU VAL PRO GLU LYS PHE ARG LYS ILE
SEQRES  28 A  713  ARG GLU ILE PRO MSE PHE ILE ILE LEU ASP SER GLY LEU
SEQRES  29 A  713  LEU ALA ASP ILE GLN ASN PHE ALA THR ASN GLU PHE ARG
SEQRES  30 A  713  GLU LEU VAL LYS SER MSE TYR TYR GLU LYS VAL ILE THR
SEQRES  31 A  713  GLU ASP LEU ASN SER ASP LYS GLY ILE ILE GLU VAL VAL
SEQRES  32 A  713  GLU GLN VAL SER SER PHE MSE LYS GLY LYS GLU LEU GLY
SEQRES  33 A  713  LEU ALA PHE ILE ALA ALA ARG ASN LYS LEU SER SER GLU
SEQRES  34 A  713  LYS PHE GLU GLU ILE LYS ARG ARG LEU PHE ASN LEU ASN
SEQRES  35 A  713  VAL ILE SER GLN VAL VAL ASN GLU ASP THR LEU LYS ASN
SEQRES  36 A  713  LYS ARG ASP LYS TYR ASP ARG ASN ARG LEU ASP LEU PHE
SEQRES  37 A  713  VAL ARG HIS ASN LEU LEU PHE GLN VAL LEU SER LYS LEU
SEQRES  38 A  713  GLY VAL LYS TYR TYR VAL LEU ASP TYR ARG PHE ASN TYR
SEQRES  39 A  713  ASP TYR ILE ILE GLY ILE ASP VAL ALA PRO MSE LYS ARG
SEQRES  40 A  713  SER GLU GLY TYR ILE GLY GLY SER ALA VAL MSE PHE ASP
SEQRES  41 A  713  SER GLN GLY TYR ILE ARG LYS ILE VAL PRO ILE LYS ILE
SEQRES  42 A  713  GLY GLU GLN ARG GLY GLU SER VAL ASP MSE ASN GLU PHE
SEQRES  43 A  713  PHE LYS GLU MSE VAL ASP LYS PHE LYS GLU PHE ASN ILE
SEQRES  44 A  713  LYS LEU ASP ASN LYS LYS ILE LEU LEU LEU ARG ASP GLY
SEQRES  45 A  713  ARG ILE THR ASN ASN GLU GLU GLU GLY LEU LYS TYR ILE
SEQRES  46 A  713  SER GLU MSE PHE ASP ILE GLU VAL VAL THR MSE ASP VAL
SEQRES  47 A  713  ILE LYS ASN HIS PRO VAL ARG ALA PHE ALA ASN MSE LYS
SEQRES  48 A  713  MSE TYR PHE ASN LEU GLY GLY ALA ILE TYR LEU ILE PRO
SEQRES  49 A  713  HIS LYS LEU LYS GLN ALA LYS GLY THR PRO ILE PRO ILE
SEQRES  50 A  713  LYS LEU ALA LYS LYS ARG ILE LLE LYS ASN GLY LYS VAL
SEQRES  51 A  713  GLU LYS GLN SER ILE THR ARG GLN ASP VAL LEU ASP ILE
SEQRES  52 A  713  PHE ILE LEU THR ARG LEU ASN TYR GLY SER ILE SER ALA
SEQRES  53 A  713  ASP MSE ARG LEU PRO ALA PRO VAL HIS TYR ALA HIS LYS
SEQRES  54 A  713  PHE ALA ASN ALA ILE ARG ASN GLU TRP LYS ILE LYS GLU
SEQRES  55 A  713  GLU PHE LEU ALA GLU GLY PHE LEU TYR PHE VAL
CRYST1   69.726  104.188   74.015  90.00 102.83  90.00 P 21           2
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.014342  0.000000  0.003265        0.00000
SCALE2      0.000000  0.009598  0.000000        0.00000
SCALE3      0.000000  0.000000  0.013857        0.00000
ATOM      1  CB  SER A   0      -9.237  31.412  15.695  1.00 52.89      A
ATOM      2  OG  SER A   0      -9.737  30.155  16.110  1.00 52.89      A
ATOM      3  C   SER A   0     -10.483  32.911  17.228  1.00 79.00      A
ATOM      4  O   SER A   0     -10.625  34.075  17.612  1.00 79.00      A
ATOM      5  N   SER A   0      -8.485  31.638  18.031  1.00 79.00      A
ATOM      6  CA  SER A   0      -9.110  32.356  16.883  1.00 79.00      A
ATOM      7  N   MSE A   1     -11.494  32.061  17.086  1.00 80.16      A
ATOM      8  CA  MSE A   1     -12.873  32.436  17.365  1.00 80.16      A
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ATOM      9  CB  MSE A   1     -13.792  31.773  16.330  1.00148.49      A
ATOM     10  CG  MSE A   1     -15.277  32.075  16.475  1.00148.49      A
ATOM     11  SE  MSE A   1     -15.681  33.960  16.497  1.00148.49      A
ATOM     12  CE  MSE A   1     -16.904  33.999  17.989  1.00148.49      A
ATOM     13  C   MSE A   1     -13.266  32.013  18.780  1.00 80.16      A
ATOM     14  O   MSE A   1     -12.455  31.466  19.529  1.00 80.16      A
ATOM     15  N   LYS A   2     -14.514  32.287  19.141  1.00 61.75      A
ATOM     16  CA  LYS A   2     -15.048  31.929  20.442  1.00 61.75      A
ATOM     17  CB  LYS A   2     -15.945  33.044  20.970  1.00 71.24      A
ATOM     18  CG  LYS A   2     -15.274  34.401  21.005  1.00 71.24      A
ATOM     19  CD  LYS A   2     -16.202  35.452  21.576  1.00 71.24      A
ATOM     20  CE  LYS A   2     -15.521  36.806  21.662  1.00 71.24      A
ATOM     21  NZ  LYS A   2     -16.416  37.829  22.282  1.00 71.24      A
ATOM     22  C   LYS A   2     -15.860  30.656  20.264  1.00 61.75      A
ATOM     23  O   LYS A   2     -16.065  30.196  19.139  1.00 61.75      A
ATOM     24  N   ALA A   3     -16.313  30.076  21.370  1.00 49.57      A
ATOM     25  CA  ALA A   3     -17.103  28.864  21.295  1.00 49.57      A
ATOM     26  CB  ALA A   3     -16.203  27.673  21.016  1.00 38.38      A
ATOM     27  C   ALA A   3     -17.859  28.681  22.597  1.00 49.57      A

ATOM     28  O   ALA A   3     -17.505  29.269  23.618  1.00 49.57      A
ATOM     29  N   ILE A   4     -18.921  27.885  22.552  1.00 48.74      A
ATOM     30  CA  ILE A   4     -19.728  27.632  23.736  1.00 48.74      A
ATOM     31  CB  ILE A   4     -21.239  27.735  23.437  1.00 52.34      A
ATOM     32  CG2 ILE A   4     -22.021  27.720  24.743  1.00 52.34      A
ATOM     33  CG1 ILE A   4     -21.545  29.034  22.677  1.00 52.34      A
ATOM     34  CD1 ILE A   4     -21.149  30.289  23.415  1.00 52.34      A
ATOM     35  C   ILE A   4     -19.433  26.223  24.218  1.00 48.74      A
ATOM     36  O   ILE A   4     -19.513  25.259  23.454  1.00 48.74      A
ATOM     37  N   VAL A   5     -19.075  26.103  25.489  1.00 41.68      A
ATOM     38  CA  VAL A   5     -18.775  24.794  26.033  1.00 41.68      A
ATOM     39  CB  VAL A   5     -17.244  24.619  26.297  1.00 47.32      A
ATOM     40  CG1 VAL A   5     -16.454  25.009  25.056  1.00 47.32      A
ATOM     41  CG2 VAL A   5     -16.802  25.455  27.483  1.00 47.32      A
ATOM     42  C   VAL A   5     -19.536  24.607  27.328  1.00 41.68      A
ATOM     43  O   VAL A   5     -19.790  25.565  28.051  1.00 41.68      A
ATOM     44  N   VAL A   6     -19.922  23.369  27.597  1.00 42.89      A
ATOM     45  CA  VAL A   6     -20.622  23.041  28.824  1.00 42.89      A
ATOM     46  CB  VAL A   6     -21.432  21.730  28.673  1.00 36.57      A
ATOM     47  CG1 VAL A   6     -22.045  21.327  30.019  1.00 36.57      A
ATOM     48  CG2 VAL A   6     -22.532  21.925  27.614  1.00 36.57      A
ATOM     49  C   VAL A   6     -19.549  22.824  29.882  1.00 42.89      A
ATOM     50  O   VAL A   6     -18.499  22.236  29.591  1.00 42.89      A
ATOM     51  N   ILE A   7     -19.802  23.308  31.095  1.00 41.08      A
ATOM     52  CA  ILE A   7     -18.856  23.138  32.197  1.00 41.08      A
ATOM     53  CB  ILE A   7     -18.278  24.496  32.676  1.00 37.86      A
ATOM     54  CG2 ILE A   7     -17.298  25.030  31.642  1.00 37.86      A
ATOM     55  CG1 ILE A   7     -19.418  25.475  32.948  1.00 37.86      A
ATOM     56  CD1 ILE A   7     -19.007  26.725  33.697  1.00 37.86      A
ATOM     57  C   ILE A   7     -19.595  22.476  33.346  1.00 41.08      A
ATOM     58  O   ILE A   7     -20.830  22.460  33.353  1.00 41.08      A
ATOM     59  N   ASN A   8     -18.847  21.949  34.318  1.00 40.94      A
ATOM     60  CA  ASN A   8     -19.443  21.253  35.460  1.00 40.94      A
ATOM     61  CB  ASN A   8     -18.456  20.201  36.002  1.00 34.10      A
ATOM     62  CG  ASN A   8     -17.200  20.807  36.637  1.00 34.10      A
ATOM     63  OD1 ASN A   8     -16.866  21.979  36.429  1.00 34.10      A
ATOM     64  ND2 ASN A   8     -16.487  19.988  37.404  1.00 34.10      A
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ATOM     65  C   ASN A   8     -19.989  22.120  36.602  1.00 40.94      A
ATOM     66  O   ASN A   8     -19.796  21.815  37.781  1.00 40.94      A
ATOM     67  N   LEU A   9     -20.689  23.190  36.239  1.00 39.65      A
ATOM     68  CA  LEU A   9     -21.307  24.102  37.198  1.00 39.65      A
ATOM     69  CB  LEU A   9     -20.774  25.537  37.038  1.00 33.69      A
ATOM     70  CG  LEU A   9     -19.433  25.989  37.614  1.00 33.69      A
ATOM     71  CD1 LEU A   9     -18.292  25.228  36.968  1.00 33.69      A
ATOM     72  CD2 LEU A   9     -19.275  27.487  37.387  1.00 33.69      A
ATOM     73  C   LEU A   9     -22.816  24.136  36.948  1.00 39.65      A
ATOM     74  O   LEU A   9     -23.280  23.929  35.821  1.00 39.65      A
ATOM     75  N   VAL A  10     -23.570  24.400  38.009  1.00 43.35      A
ATOM     76  CA  VAL A  10     -25.011  24.503  37.921  1.00 43.35      A
ATOM     77  CB  VAL A  10     -25.728  23.223  38.435  1.00 52.91      A
ATOM     78  CG1 VAL A  10     -25.372  22.949  39.880  1.00 52.91      A
ATOM     79  CG2 VAL A  10     -27.219  23.389  38.298  1.00 52.91      A
ATOM     80  C   VAL A  10     -25.409  25.702  38.770  1.00 43.35      A
ATOM     81  O   VAL A  10     -25.005  25.821  39.935  1.00 43.35      A
ATOM     82  N   LYS A  11     -26.191  26.595  38.175  1.00 45.06      A
ATOM     83  CA  LYS A  11     -26.634  27.794  38.862  1.00 45.06      A
ATOM     84  CB  LYS A  11     -27.457  28.667  37.913  1.00 61.94      A
ATOM     85  CG  LYS A  11     -27.732  30.067  38.450  1.00 61.94      A
ATOM     86  CD  LYS A  11     -28.623  30.840  37.503  1.00 61.94      A
ATOM     87  CE  LYS A  11     -29.030  32.183  38.076  1.00 61.94      A
ATOM     88  NZ  LYS A  11     -30.076  32.817  37.209  1.00 61.94      A
ATOM     89  C   LYS A  11     -27.444  27.494  40.119  1.00 45.06      A
ATOM     90  O   LYS A  11     -28.290  26.604  40.140  1.00 45.06      A
ATOM     91  N   ILE A  12     -27.181  28.252  41.171  1.00 38.81      A
ATOM     92  CA  ILE A  12     -27.895  28.081  42.433  1.00 38.81      A
ATOM     93  CB  ILE A  12     -26.921  28.253  43.618  1.00 40.09      A
ATOM     94  CG2 ILE A  12     -27.682  28.230  44.927  1.00 40.09      A
ATOM     95  CG1 ILE A  12     -25.846  27.160  43.563  1.00 40.09      A
ATOM     96  CD1 ILE A  12     -24.656  27.420  44.491  1.00 40.09      A
ATOM     97  C   ILE A  12     -28.986  29.157  42.509  1.00 38.81      A
ATOM     98  O   ILE A  12     -28.744  30.311  42.152  1.00 38.81      A
ATOM     99  N   ASN A  13     -30.177  28.793  42.968  1.00 47.45      A
ATOM    100  CA  ASN A  13     -31.263  29.771  43.061  1.00 47.45      A
ATOM    101  CB  ASN A  13     -32.602  29.078  43.307  1.00 60.49      A
ATOM    102  CG  ASN A  13     -33.781  30.010  43.089  1.00 60.49      A
ATOM    103  OD1 ASN A  13     -34.493  29.907  42.090  1.00 60.49      A
ATOM    104  ND2 ASN A  13     -33.981  30.938  44.014  1.00 60.49      A
ATOM    105  C   ASN A  13     -30.993  30.751  44.201  1.00 47.45      A
ATOM    106  O   ASN A  13     -30.650  30.336  45.305  1.00 47.45      A
ATOM    107  N   LYS A  14     -31.177  32.043  43.932  1.00 50.64      A
ATOM    108  CA  LYS A  14     -30.930  33.087  44.921  1.00 50.64      A
ATOM    109  CB  LYS A  14     -31.128  34.473  44.300  1.00 99.82      A
ATOM    110  CG  LYS A  14     -32.582  34.855  44.063  1.00 99.82      A
ATOM    111  CD  LYS A  14     -32.700  36.281  43.541  1.00 99.82      A
ATOM    112  CE  LYS A  14     -34.152  36.663  43.289  1.00 99.82      A
ATOM    113  NZ  LYS A  14     -34.268  38.033  42.713  1.00 99.82      A
ATOM    114  C   LYS A  14     -31.802  32.972  46.167  1.00 50.64      A
ATOM    115  O   LYS A  14     -31.497  33.563  47.201  1.00 50.64      A
ATOM    116  N   LYS A  15     -32.883  32.213  46.084  1.00 59.16      A
ATOM    117  CA  LYS A  15     -33.751  32.069  47.240  1.00 59.16      A
ATOM    118  CB  LYS A  15     -35.048  31.347  46.856  1.00 77.44      A
ATOM    119  CG  LYS A  15     -34.907  29.861  46.563  1.00 77.44      A
ATOM    120  CD  LYS A  15     -36.283  29.239  46.347  1.00 77.44      A
ATOM    121  CE  LYS A  15     -36.210  27.732  46.172  1.00 77.44      A
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ATOM    122  NZ  LYS A  15     -37.577  27.136  46.125  1.00 77.44      A
ATOM    123  C   LYS A  15     -33.042  31.316  48.365  1.00 59.16      A
ATOM    124  O   LYS A  15     -33.580  31.178  49.467  1.00 59.16      A
ATOM    125  N   ILE A  16     -31.834  30.825  48.095  1.00 58.05      A
ATOM    126  CA  ILE A  16     -31.089  30.105  49.123  1.00 58.05      A
ATOM    127  CB  ILE A  16     -30.008  29.171  48.513  1.00 56.10      A
ATOM    128  CG2 ILE A  16     -28.900  29.990  47.868  1.00 56.10      A
ATOM    129  CG1 ILE A  16     -29.429  28.281  49.614  1.00 56.10      A
ATOM    130  CD1 ILE A  16     -28.387  27.287  49.147  1.00 56.10      A
ATOM    131  C   ILE A  16     -30.413  31.101  50.062  1.00 58.05      A
ATOM    132  O   ILE A  16     -30.199  30.817  51.238  1.00 58.05      A
ATOM    133  N   ILE A  17     -30.084  32.274  49.531  1.00 60.10      A
ATOM    134  CA  ILE A  17     -29.440  33.314  50.317  1.00 60.10      A
ATOM    135  CB  ILE A  17     -29.332  34.611  49.481  1.00 48.50      A
ATOM    136  CG2 ILE A  17     -28.759  35.748  50.319  1.00 48.50      A
ATOM    137  CG1 ILE A  17     -28.445  34.335  48.256  1.00 48.50      A
ATOM    138  CD1 ILE A  17     -28.312  35.487  47.310  1.00 48.50      A
ATOM    139  C   ILE A  17     -30.251  33.522  51.600  1.00 60.10      A
ATOM    140  O   ILE A  17     -31.474  33.669  51.562  1.00 60.10      A
ATOM    141  N   PRO A  18     -29.573  33.517  52.759  1.00 61.75      A
ATOM    142  CD  PRO A  18     -28.105  33.488  52.895  1.00 41.72      A
ATOM    143  CA  PRO A  18     -30.211  33.688  54.067  1.00 61.75      A
ATOM    144  CB  PRO A  18     -29.136  33.201  55.030  1.00 41.72      A
ATOM    145  CG  PRO A  18     -27.889  33.752  54.392  1.00 41.72      A
ATOM    146  C   PRO A  18     -30.654  35.112  54.376  1.00 61.75      A
ATOM    147  O   PRO A  18     -29.958  36.074  54.055  1.00 61.75      A
ATOM    148  N   ASP A  19     -31.812  35.229  55.016  1.00101.98      A
ATOM    149  CA  ASP A  19     -32.359  36.525  55.389  1.00101.98      A
ATOM    150  CB  ASP A  19     -33.726  36.344  56.053  1.00121.69      A
ATOM    151  CG  ASP A  19     -34.729  35.656  55.146  1.00121.69      A
ATOM    152  OD1 ASP A  19     -35.052  36.221  54.080  1.00121.69      A
ATOM    153  OD2 ASP A  19     -35.191  34.549  55.498  1.00121.69      A
ATOM    154  C   ASP A  19     -31.410  37.244  56.345  1.00101.98      A
ATOM    155  O   ASP A  19     -31.004  38.379  56.088  1.00101.98      A

ATOM    156  N   LYS A  20     -31.053  36.580  57.442  1.00 78.31      A
ATOM    157  CA  LYS A  20     -30.150  37.176  58.424  1.00 78.31      A
ATOM    158  CB  LYS A  20     -30.921  37.581  59.690  1.00113.24      A
ATOM    159  CG  LYS A  20     -31.956  36.578  60.185  1.00113.24      A
ATOM    160  CD  LYS A  20     -33.246  36.672  59.382  1.00113.24      A
ATOM    161  CE  LYS A  20     -34.345  35.798  59.972  1.00113.24      A
ATOM    162  NZ  LYS A  20     -34.762  36.244  61.333  1.00113.24      A
ATOM    163  C   LYS A  20     -28.948  36.315  58.814  1.00 78.31      A
ATOM    164  O   LYS A  20     -29.064  35.109  59.018  1.00 78.31      A
ATOM    165  N   ILE A  21     -27.793  36.966  58.907  1.00 95.36      A
ATOM    166  CA  ILE A  21     -26.539  36.323  59.282  1.00 95.36      A
ATOM    167  CB  ILE A  21     -25.423  36.637  58.251  1.00 57.51      A
ATOM    168  CG2 ILE A  21     -24.108  36.017  58.699  1.00 57.51      A
ATOM    169  CG1 ILE A  21     -25.824  36.121  56.866  1.00 57.51      A
ATOM    170  CD1 ILE A  21     -24.886  36.563  55.756  1.00 57.51      A
ATOM    171  C   ILE A  21     -26.128  36.891  60.644  1.00 95.36      A
ATOM    172  O   ILE A  21     -26.275  38.087  60.890  1.00 95.36      A
ATOM    173  N   TYR A  22     -25.614  36.037  61.522  1.00 81.78      A
ATOM    174  CA  TYR A  22     -25.198  36.469  62.854  1.00 81.78      A
ATOM    175  CB  TYR A  22     -25.946  35.663  63.916  1.00 76.11      A
ATOM    176  CG  TYR A  22     -27.447  35.661  63.739  1.00 76.11      A
ATOM    177  CD1 TYR A  22     -28.228  36.741  64.161  1.00 76.11      A
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FIGURE 25 CON'T
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ATOM	178	CE1	TYR	A	22	-29.616	36.741	63.985	1.00	76.11	A
ATOM	179	CD2	TYR	A	22	-28.089	34.585	63.136	1.00	76.11	A
ATOM	180	CE2	TYR	A	22	-29.469	34.575	62.955	1.00	76.11	A
ATOM	181	CZ	TYR	A	22	-30.227	35.653	63.380	1.00	76.11	A
ATOM	182	OH	TYR	A	22	-31.590	35.631	63.195	1.00	76.11	A
ATOM	183	C	TYR	A	22	-23.694	36.297	63.054	1.00	81.78	A
ATOM	184	O	TYR	A	22	-23.164	35.194	62.903	1.00	81.78	A
ATOM	185	N	VAL	A	23	-23.010	37.387	63.392	1.00	68.96	A
ATOM	186	CA	VAL	A	23	-21.569	37.339	63.619	1.00	68.96	A
ATOM	187	CB	VAL	A	23	-20.882	38.654	63.200	1.00	64.65	A
ATOM	188	CG1	VAL	A	23	-19.374	38.532	63.374	1.00	64.65	A
ATOM	189	CG2	VAL	A	23	-21.217	38.983	61.755	1.00	64.65	A
ATOM	190	C	VAL	A	23	-21.297	37.095	65.099	1.00	68.96	A
ATOM	191	O	VAL	A	23	-21.990	37.639	65.961	1.00	68.96	A
ATOM	192	N	TYR	A	24	-20.293	36.267	65.386	1.00	73.51	A
ATOM	193	CA	TYR	A	24	-19.922	35.936	66.759	1.00	73.51	A
ATOM	194	CB	TYR	A	24	-20.523	34.586	67.167	1.00	84.13	A
ATOM	195	CG	TYR	A	24	-22.035	34.525	67.153	1.00	84.13	A
ATOM	196	CD1	TYR	A	24	-22.788	35.069	68.193	1.00	84.13	A
ATOM	197	CE1	TYR	A	24	-24.183	34.998	68.185	1.00	84.13	A
ATOM	198	CD2	TYR	A	24	-22.713	33.911	66.101	1.00	84.13	A
ATOM	199	CE2	TYR	A	24	-24.100	33.837	66.081	1.00	84.13	A
ATOM	200	CZ	TYR	A	24	-24.830	34.379	67.125	1.00	84.13	A
ATOM	201	OH	TYR	A	24	-26.204	34.273	67.115	1.00	84.13	A
ATOM	202	C	TYR	A	24	-18.403	35.866	66.917	1.00	73.51	A
ATOM	203	O	TYR	A	24	-17.672	35.607	65.956	1.00	73.51	A
ATOM	204	N	ARG	A	25	-17.938	36.125	68.112	1.00	93.64	A
ATOM	205	CA	ARG	A	25	-16.546	36.084	68.363	1.00	93.64	A
ATOM	206	CB	ARG	A	25	-15.884	37.479	68.516	1.00	79.47	A
ATOM	207	CG	ARG	A	25	-14.571	37.477	69.294	1.00	79.47	A
ATOM	208	CD	ARG	A	25	-14.237	38.857	69.837	1.00	79.47	A
ATOM	209	NE	ARG	A	25	-14.234	39.853	68.771	1.00	79.47	A
ATOM	210	CZ	ARG	A	25	-13.304	39.964	67.829	1.00	79.47	A
ATOM	211	NH1	ARG	A	25	-12.264	39.140	67.824	1.00	79.47	A
ATOM	212	NH2	ARG	A	25	-13.417	40.895	66.887	1.00	79.47	A
ATOM	213	C	ARG	A	25	-16.396	35.380	69.651	1.00	93.64	A
ATOM	214	O	ARG	A	25	-17.187	35.516	70.592	1.00	93.64	A
ATOM	215	N	LEU	A	26	-15.390	34.593	69.644	1.00	100.08	A
ATOM	216	CA	LEU	A	26	-14.941	33.836	70.734	1.00	100.08	A
ATOM	217	CB	LEU	A	26	-14.890	32.337	70.424	1.00	106.38	A
ATOM	218	CG	LEU	A	26	-16.199	31.672	69.939	1.00	106.38	A
ATOM	219	CD1	LEU	A	26	-15.940	30.278	69.378	1.00	106.38	A
ATOM	220	CD2	LEU	A	26	-17.209	31.596	71.075	1.00	106.38	A
ATOM	221	C	LEU	A	26	-13.537	34.319	71.039	1.00	100.08	A
ATOM	222	O	LEU	A	26	-12.996	34.050	72.115	1.00	100.08	A
ATOM	223	N	TYR	A	39	-14.455	18.230	68.139	1.00	123.30	A
ATOM	224	CA	TYR	A	39	-15.122	19.523	68.054	1.00	123.30	A
ATOM	225	CB	TYR	A	39	-15.739	19.886	69.404	1.00	114.29	A
ATOM	226	CG	TYR	A	39	-17.000	20.711	69.308	1.00	114.29	A
ATOM	227	CD1	TYR	A	39	-18.197	20.134	68.886	1.00	114.29	A
ATOM	228	CE1	TYR	A	39	-19.366	20.880	68.802	1.00	114.29	A
ATOM	229	CD2	TYR	A	39	-17.003	22.064	69.642	1.00	114.29	A
ATOM	230	CE2	TYR	A	39	-18.171	22.823	69.560	1.00	114.29	A
ATOM	231	CZ	TYR	A	39	-19.348	22.223	69.139	1.00	114.29	A
ATOM	232	OH	TYR	A	39	-20.507	22.961	69.053	1.00	114.29	A
ATOM	233	C	TYR	A	39	-14.105	20.589	67.663	1.00	123.30	A
ATOM	234	O	TYR	A	39	-12.899	20.341	67.693	1.00	123.30	A

ATOM	235	N	SER	A	40	-14.594	21.772	67.303	1.00	68.80	A
ATOM	236	CA	SER	A	40	-13.726	22.883	66.910	1.00	68.80	A
ATOM	237	CB	SER	A	40	-12.844	22.493	65.722	1.00	73.40	A
ATOM	238	OG	SER	A	40	-13.623	22.334	64.548	1.00	73.40	A
ATOM	239	C	SER	A	40	-14.564	24.094	66.519	1.00	68.80	A
ATOM	240	O	SER	A	40	-15.795	24.045	66.549	1.00	68.80	A
ATOM	241	N	ILE	A	41	-13.885	25.176	66.149	1.00	89.34	A
ATOM	242	CA	ILE	A	41	-14.556	26.407	65.747	1.00	89.34	A
ATOM	243	CB	ILE	A	41	-13.568	27.590	65.691	1.00	64.37	A
ATOM	244	CG2	ILE	A	41	-12.487	27.320	64.657	1.00	64.37	A
ATOM	245	CG1	ILE	A	41	-14.319	28.877	65.353	1.00	64.37	A
ATOM	246	CD1	ILE	A	41	-13.425	30.082	65.224	1.00	64.37	A
ATOM	247	C	ILE	A	41	-15.194	26.236	64.372	1.00	89.34	A
ATOM	248	O	ILE	A	41	-16.176	26.903	64.047	1.00	89.34	A
ATOM	249	N	TYR	A	42	-14.621	25.342	63.570	1.00	72.02	A
ATOM	250	CA	TYR	A	42	-15.133	25.058	62.235	1.00	72.02	A
ATOM	251	CB	TYR	A	42	-14.070	24.330	61.408	1.00	83.35	A
ATOM	252	CG	TYR	A	42	-13.024	25.237	60.793	1.00	83.35	A
ATOM	253	CD1	TYR	A	42	-13.329	26.036	59.692	1.00	83.35	A
ATOM	254	CE1	TYR	A	42	-12.365	26.862	59.107	1.00	83.35	A
ATOM	255	CD2	TYR	A	42	-11.726	25.286	61.303	1.00	83.35	A
ATOM	256	CE2	TYR	A	42	-10.753	26.107	60.727	1.00	83.35	A
ATOM	257	CZ	TYR	A	42	-11.079	26.892	59.630	1.00	83.35	A
ATOM	258	OH	TYR	A	42	-10.124	27.703	59.056	1.00	83.35	A
ATOM	259	C	TYR	A	42	-16.383	24.196	62.357	1.00	72.02	A
ATOM	260	O	TYR	A	42	-17.345	24.360	61.603	1.00	72.02	A
ATOM	261	N	ARG	A	43	-16.361	23.278	63.317	1.00	72.78	A
ATOM	262	CA	ARG	A	43	-17.490	22.393	63.554	1.00	72.78	A
ATOM	263	CB	ARG	A	43	-17.069	21.203	64.419	1.00	148.84	A
ATOM	264	CG	ARG	A	43	-16.039	20.305	63.761	1.00	148.84	A
ATOM	265	CD	ARG	A	43	-15.670	19.134	64.650	1.00	148.84	A
ATOM	266	NE	ARG	A	43	-14.622	18.315	64.049	1.00	148.84	A
ATOM	267	CZ	ARG	A	43	-14.085	17.245	64.626	1.00	148.84	A
ATOM	268	NH1	ARG	A	43	-14.498	16.857	65.825	1.00	148.84	A
ATOM	269	NH2	ARG	A	43	-13.134	16.561	64.003	1.00	148.84	A
ATOM	270	C	ARG	A	43	-18.597	23.165	64.246	1.00	72.78	A
ATOM	271	O	ARG	A	43	-19.780	22.869	64.060	1.00	72.78	A
ATOM	272	N	LEU	A	44	-18.212	24.150	65.054	1.00	60.26	A
ATOM	273	CA	LEU	A	44	-19.198	24.967	65.754	1.00	60.26	A
ATOM	274	CB	LEU	A	44	-18.508	25.953	66.699	1.00	68.35	A
ATOM	275	CG	LEU	A	44	-19.425	26.990	67.354	1.00	68.35	A
ATOM	276	CD1	LEU	A	44	-20.435	26.291	68.256	1.00	68.35	A
ATOM	277	CD2	LEU	A	44	-18.589	27.988	68.142	1.00	68.35	A
ATOM	278	C	LEU	A	44	-19.981	25.729	64.695	1.00	60.26	A
ATOM	279	O	LEU	A	44	-21.208	25.618	64.598	1.00	60.26	A
ATOM	280	N	ALA	A	45	-19.249	26.493	63.892	1.00	60.85	A
ATOM	281	CA	ALA	A	45	-19.836	27.276	62.812	1.00	60.85	A
ATOM	282	CB	ALA	A	45	-18.726	27.876	61.957	1.00	58.80	A
ATOM	283	C	ALA	A	45	-20.747	26.398	61.954	1.00	60.85	A
ATOM	284	O	ALA	A	45	-21.842	26.812	61.576	1.00	60.85	A
ATOM	285	N	TYR	A	46	-20.289	25.177	61.670	1.00	63.28	A
ATOM	286	CA	TYR	A	46	-21.034	24.219	60.850	1.00	63.28	A
ATOM	287	CB	TYR	A	46	-20.171	22.985	60.559	1.00	63.27	A
ATOM	288	CG	TYR	A	46	-20.869	21.954	59.700	1.00	63.27	A
ATOM	289	CD1	TYR	A	46	-20.767	21.998	58.308	1.00	63.27	A
ATOM	290	CE1	TYR	A	46	-21.452	21.090	57.505	1.00	63.27	A

ATOM	291	CD2	TYR	A	46	-21.675	20.971	60.270	1.00	63.27	A
ATOM	292	CE2	TYR	A	46	-22.370	20.060	59.475	1.00	63.27	A
ATOM	293	CZ	TYR	A	46	-22.250	20.130	58.092	1.00	63.27	A
ATOM	294	OH	TYR	A	46	-22.933	19.246	57.296	1.00	63.27	A
ATOM	295	C	TYR	A	46	-22.341	23.748	61.476	1.00	63.28	A
ATOM	296	O	TYR	A	46	-23.380	23.700	60.807	1.00	63.28	A
ATOM	297	N	GLU	A	47	-22.283	23.370	62.751	1.00	72.26	A
ATOM	298	CA	GLU	A	47	-23.469	22.884	63.454	1.00	72.26	A
ATOM	299	CB	GLU	A	47	-23.085	22.355	64.839	1.00	120.38	A
ATOM	300	CG	GLU	A	47	-22.106	21.188	64.792	1.00	120.38	A
ATOM	301	CD	GLU	A	47	-21.873	20.556	66.151	1.00	120.38	A
ATOM	302	OE1	GLU	A	47	-21.515	21.287	67.097	1.00	120.38	A
ATOM	303	OE2	GLU	A	47	-22.043	19.324	66.271	1.00	120.38	A
ATOM	304	C	GLU	A	47	-24.540	23.963	63.575	1.00	72.26	A
ATOM	305	O	GLU	A	47	-25.725	23.661	63.701	1.00	72.26	A
ATOM	306	N	ASN	A	48	-24.120	25.222	63.524	1.00	83.72	A
ATOM	307	CA	ASN	A	48	-25.059	26.333	63.611	1.00	83.72	A
ATOM	308	CB	ASN	A	48	-24.462	27.458	64.467	1.00	71.59	A
ATOM	309	CG	ASN	A	48	-24.410	27.102	65.950	1.00	71.59	A
ATOM	310	OD1	ASN	A	48	-25.445	26.991	66.613	1.00	71.59	A
ATOM	311	ND2	ASN	A	48	-23.203	26.917	66.473	1.00	71.59	A
ATOM	312	C	ASN	A	48	-25.415	26.854	62.211	1.00	83.72	A
ATOM	313	O	ASN	A	48	-25.897	27.975	62.058	1.00	83.72	A
ATOM	314	N	VAL	A	49	-25.188	26.026	61.194	1.00	69.39	A
ATOM	315	CA	VAL	A	49	-25.479	26.409	59.815	1.00	69.39	A
ATOM	316	CB	VAL	A	49	-26.996	26.575	59.573	1.00	62.36	A
ATOM	317	CG1	VAL	A	49	-27.275	26.655	58.075	1.00	62.36	A
ATOM	318	CG2	VAL	A	49	-27.754	25.410	60.193	1.00	62.36	A
ATOM	319	C	VAL	A	49	-24.791	27.734	59.520	1.00	69.39	A
ATOM	320	O	VAL	A	49	-25.437	28.729	59.187	1.00	69.39	A
ATOM	321	N	GLY	A	50	-23.471	27.734	59.653	1.00	52.70	A
ATOM	322	CA	GLY	A	50	-22.699	28.932	59.412	1.00	52.70	A
ATOM	323	C	GLY	A	50	-21.288	28.562	59.012	1.00	52.70	A
ATOM	324	O	GLY	A	50	-20.981	27.379	58.832	1.00	52.70	A
ATOM	325	N	ILE	A	51	-20.435	29.570	58.874	1.00	58.71	A
ATOM	326	CA	ILE	A	51	-19.049	29.365	58.489	1.00	58.71	A
ATOM	327	CB	ILE	A	51	-18.829	29.759	56.999	1.00	69.06	A
ATOM	328	CG2	ILE	A	51	-19.485	28.727	56.089	1.00	69.06	A
ATOM	329	CG1	ILE	A	51	-19.441	31.134	56.703	1.00	69.06	A
ATOM	330	CD1	ILE	A	51	-18.710	32.291	57.315	1.00	69.06	A
ATOM	331	C	ILE	A	51	-18.096	30.157	59.380	1.00	58.71	A
ATOM	332	O	ILE	A	51	-18.528	30.830	60.322	1.00	58.71	A
ATOM	333	N	VAL	A	52	-16.801	30.069	59.078	1.00	74.42	A
ATOM	334	CA	VAL	A	52	-15.767	30.772	59.836	1.00	74.42	A
ATOM	335	CB	VAL	A	52	-14.562	29.844	60.141	1.00	62.30	A
ATOM	336	CG1	VAL	A	52	-13.472	30.618	60.874	1.00	62.30	A
ATOM	337	CG2	VAL	A	52	-15.016	28.659	60.975	1.00	62.30	A
ATOM	338	C	VAL	A	52	-15.266	31.967	59.030	1.00	74.42	A
ATOM	339	O	VAL	A	52	-14.822	31.810	57.890	1.00	74.42	A
ATOM	340	N	ILE	A	53	-15.343	33.157	59.622	1.00	97.43	A
ATOM	341	CA	ILE	A	53	-14.903	34.381	58.956	1.00	97.43	A
ATOM	342	CB	ILE	A	53	-15.704	35.608	59.445	1.00	108.88	A
ATOM	343	CG2	ILE	A	53	-15.135	36.879	58.828	1.00	108.88	A
ATOM	344	CG1	ILE	A	53	-17.180	35.453	59.077	1.00	108.88	A
ATOM	345	CD1	ILE	A	53	-18.044	36.623	59.513	1.00	108.88	A
ATOM	346	C	ILE	A	53	-13.421	34.668	59.177	1.00	97.43	A
ATOM	347	O	ILE	A	53	-12.657	34.796	58.221	1.00	97.43	A

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ATOM    348  N   ASP A  54     -13.024  34.778  60.441  1.00 84.01      A
ATOM    349  CA  ASP A  54     -11.635  35.058  60.785  1.00 84.01      A
ATOM    350  CB  ASP A  54     -11.544  36.381  61.555  1.00 79.35      A
ATOM    351  CG  ASP A  54     -10.156  36.999  61.499  1.00 79.35      A
ATOM    352  OD1 ASP A  54      -9.165  36.277  61.745  1.00 79.35      A
ATOM    353  OD2 ASP A  54     -10.058  38.212  61.214  1.00 79.35      A
ATOM    354  C   ASP A  54     -11.079  33.917  61.641  1.00 84.01      A
ATOM    355  O   ASP A  54     -11.320  33.861  62.848  1.00 84.01      A
ATOM    356  N   PRO A  55     -10.332  32.988  61.020  1.00 99.05      A
ATOM    357  CD  PRO A  55     -10.006  32.935  59.584  1.00107.30      A
ATOM    358  CA  PRO A  55      -9.742  31.845  61.725  1.00 99.05      A
ATOM    359  CB  PRO A  55      -8.938  31.145  60.632  1.00107.30      A
ATOM    360  CG  PRO A  55      -9.698  31.474  59.387  1.00107.30      A
ATOM    361  C   PRO A  55      -8.856  32.298  62.886  1.00 99.05      A
ATOM    362  O   PRO A  55      -8.745  31.615  63.906  1.00 99.05      A
ATOM    363  N   GLU A  56      -8.225  33.455  62.715  1.00113.58      A
ATOM    364  CA  GLU A  56      -7.348  34.009  63.738  1.00113.58      A
ATOM    365  CB  GLU A  56      -6.589  35.221  63.187  1.00129.86      A
ATOM    366  CG  GLU A  56      -6.240  35.137  61.708  1.00129.86      A
ATOM    367  CD  GLU A  56      -5.482  33.875  61.350  1.00129.86      A
ATOM    368  OE1 GLU A  56      -4.412  33.630  61.946  1.00129.86      A
ATOM    369  OE2 GLU A  56      -5.958  33.128  60.469  1.00129.86      A
ATOM    370  C   GLU A  56      -8.185  34.449  64.934  1.00113.58      A
ATOM    371  O   GLU A  56      -8.154  33.829  65.997  1.00113.58      A
ATOM    372  N   ASN A  57      -8.941  35.524  64.734  1.00 99.99      A
ATOM    373  CA  ASN A  57      -9.791  36.098  65.768  1.00 99.99      A
ATOM    374  CB  ASN A  57     -10.204  37.512  65.353  1.00110.57      A
ATOM    375  CG  ASN A  57      -9.010  38.419  65.105  1.00110.57      A
ATOM    376  OD1 ASN A  57      -8.276  38.767  66.032  1.00110.57      A
ATOM    377  ND2 ASN A  57      -8.806  38.800  63.848  1.00110.57      A
ATOM    378  C   ASN A  57     -11.037  35.270  66.085  1.00 99.99      A
ATOM    379  O   ASN A  57     -11.990  35.782  66.673  1.00 99.99      A
ATOM    380  N   LEU A  58     -11.024  33.998  65.698  1.00 78.90      A
ATOM    381  CA  LEU A  58     -12.148  33.096  65.946  1.00 78.90      A
ATOM    382  CB  LEU A  58     -12.103  32.589  67.392  1.00 92.24      A
ATOM    383  CG  LEU A  58     -10.853  31.837  67.851  1.00 92.24      A
ATOM    384  CD1 LEU A  58     -10.982  31.496  69.327  1.00 92.24      A
ATOM    385  CD2 LEU A  58     -10.675  30.571  67.027  1.00 92.24      A
ATOM    386  C   LEU A  58     -13.510  33.748  65.683  1.00 78.90      A
ATOM    387  O   LEU A  58     -14.413  33.681  66.520  1.00 78.90      A
ATOM    388  N   ILE A  59     -13.654  34.375  64.520  1.00 74.85      A
ATOM    389  CA  ILE A  59     -14.907  35.034  64.159  1.00 74.85      A
ATOM    390  CB  ILE A  59     -14.642  36.384  63.466  1.00 89.43      A
ATOM    391  CG2 ILE A  59     -15.963  37.062  63.121  1.00 89.43      A
ATOM    392  CG1 ILE A  59     -13.800  37.275  64.384  1.00 89.43      A
ATOM    393  CD1 ILE A  59     -13.414  38.605  63.770  1.00 89.43      A
ATOM    394  C   ILE A  59     -15.741  34.160  63.230  1.00 74.85      A
ATOM    395  O   ILE A  59     -15.301  33.806  62.141  1.00 74.85      A
ATOM    396  N   ILE A  60     -16.945  33.812  63.671  1.00 64.45      A
ATOM    397  CA  ILE A  60     -17.840  32.978  62.879  1.00 64.45      A
ATOM    398  CB  ILE A  60     -18.218  31.689  63.639  1.00 62.85      A
ATOM    399  CG2 ILE A  60     -16.955  30.962  64.093  1.00 62.85      A
ATOM    400  CG1 ILE A  60     -19.089  32.031  64.845  1.00 62.85      A
ATOM    401  CD1 ILE A  60     -19.587  30.816  65.591  1.00 62.85      A
ATOM    402  C   ILE A  60     -19.131  33.706  62.508  1.00 64.45      A
ATOM    403  O   ILE A  60     -19.567  34.619  63.211  1.00 64.45      A
ATOM    404  N   ALA A  61     -19.732  33.289  61.397  1.00 67.87      A
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ATOM	405	CA	ALA	A	61	-20.981	33.863	60.909	1.00 67.87	A
ATOM	406	CB	ALA	A	61	-20.760	34.517	59.552	1.00 50.62	A
ATOM	407	C	ALA	A	61	-21.990	32.723	60.799	1.00 67.87	A
ATOM	408	O	ALA	A	61	-21.765	31.747	60.085	1.00 67.87	A
ATOM	409	N	THR	A	62	-23.104	32.855	61.505	1.00 76.91	A
ATOM	410	CA	THR	A	62	-24.134	31.824	61.536	1.00 76.91	A
ATOM	411	CB	THR	A	62	-24.341	31.368	62.989	1.00 83.13	A
ATOM	412	OG1	THR	A	62	-23.140	30.755	63.470	1.00 83.13	A
ATOM	413	CG2	THR	A	62	-25.483	30.396	63.095	1.00 83.13	A
ATOM	414	C	THR	A	62	-25.467	32.315	60.976	1.00 76.91	A
ATOM	415	O	THR	A	62	-25.749	33.509	61.013	1.00 76.91	A
ATOM	416	N	THR	A	63	-26.282	31.401	60.450	1.00 74.40	A
ATOM	417	CA	THR	A	63	-27.588	31.788	59.922	1.00 74.40	A
ATOM	418	CB	THR	A	63	-27.928	31.099	58.568	1.00 65.90	A
ATOM	419	OG1	THR	A	63	-28.085	29.691	58.763	1.00 65.90	A
ATOM	420	CG2	THR	A	63	-26.835	31.347	57.551	1.00 65.90	A
ATOM	421	C	THR	A	63	-28.669	31.410	60.928	1.00 74.40	A
ATOM	422	O	THR	A	63	-29.852	31.642	60.693	1.00 74.40	A
ATOM	423	N	LYS	A	64	-28.253	30.826	62.048	1.00 78.25	A
ATOM	424	CA	LYS	A	64	-29.181	30.414	63.100	1.00 78.25	A
ATOM	425	CB	LYS	A	64	-29.253	28.885	63.188	1.00112.19	A
ATOM	426	CG	LYS	A	64	-29.890	28.206	61.987	1.00112.19	A
ATOM	427	CD	LYS	A	64	-31.329	28.658	61.789	1.00112.19	A
ATOM	428	CE	LYS	A	64	-32.007	27.881	60.670	1.00112.19	A
ATOM	429	NZ	LYS	A	64	-32.095	26.429	60.987	1.00112.19	A
ATOM	430	C	LYS	A	64	-28.763	30.970	64.455	1.00 78.25	A
ATOM	431	O	LYS	A	64	-27.661	31.492	64.608	1.00 78.25	A
ATOM	432	N	GLU	A	65	-29.655	30.855	65.434	1.00 99.21	A
ATOM	433	CA	GLU	A	65	-29.379	31.333	66.785	1.00 99.21	A
ATOM	434	CB	GLU	A	65	-30.639	31.217	67.649	1.00164.67	A
ATOM	435	CG	GLU	A	65	-30.475	31.723	69.076	1.00164.67	A
ATOM	436	CD	GLU	A	65	-31.782	31.725	69.849	1.00164.67	A
ATOM	437	OE1	GLU	A	65	-32.708	32.463	69.450	1.00164.67	A
ATOM	438	OE2	GLU	A	65	-31.884	30.990	70.853	1.00164.67	A
ATOM	439	C	GLU	A	65	-28.250	30.493	67.378	1.00 99.21	A
ATOM	440	O	GLU	A	65	-28.429	29.310	67.675	1.00 99.21	A
ATOM	441	N	LEU	A	66	-27.088	31.115	67.548	1.00 89.99	A
ATOM	442	CA	LEU	A	66	-25.912	30.432	68.077	1.00 89.99	A
ATOM	443	CB	LEU	A	66	-24.745	31.421	68.202	1.00 81.73	A
ATOM	444	CG	LEU	A	66	-23.378	30.947	68.716	1.00 81.73	A
ATOM	445	CD1	LEU	A	66	-23.413	30.787	70.217	1.00 81.73	A
ATOM	446	CD2	LEU	A	66	-22.991	29.639	68.046	1.00 81.73	A
ATOM	447	C	LEU	A	66	-26.114	29.724	69.409	1.00 89.99	A
ATOM	448	O	LEU	A	66	-26.455	30.351	70.412	1.00 89.99	A
ATOM	449	N	GLU	A	67	-25.902	28.411	69.406	1.00111.99	A
ATOM	450	CA	GLU	A	67	-26.008	27.608	70.618	1.00111.99	A
ATOM	451	CB	GLU	A	67	-26.849	26.351	70.389	1.00122.10	A
ATOM	452	CG	GLU	A	67	-28.325	26.602	70.159	1.00122.10	A
ATOM	453	CD	GLU	A	67	-29.129	25.316	70.173	1.00122.10	A
ATOM	454	OE1	GLU	A	67	-28.814	24.407	69.374	1.00122.10	A
ATOM	455	OE2	GLU	A	67	-30.073	25.212	70.984	1.00122.10	A
ATOM	456	C	GLU	A	67	-24.587	27.201	70.977	1.00111.99	A
ATOM	457	O	GLU	A	67	-23.938	26.464	70.236	1.00111.99	A
ATOM	458	N	TYR	A	68	-24.103	27.693	72.109	1.00 96.00	A
ATOM	459	CA	TYR	A	68	-22.752	27.388	72.549	1.00 96.00	A
ATOM	460	CB	TYR	A	68	-21.766	28.291	71.809	1.00 74.64	A

ATOM	461	CG	TYR	A	68	-20.315	28.081	72.163	1.00	74.64	A
ATOM	462	CD1	TYR	A	68	-19.759	26.800	72.202	1.00	74.64	A
ATOM	463	CE1	TYR	A	68	-18.412	26.612	72.503	1.00	74.64	A
ATOM	464	CD2	TYR	A	68	-19.488	29.168	72.434	1.00	74.64	A
ATOM	465	CE2	TYR	A	68	-18.145	28.992	72.736	1.00	74.64	A
ATOM	466	CZ	TYR	A	68	-17.612	27.716	72.769	1.00	74.64	A
ATOM	467	OH	TYR	A	68	-16.278	27.556	73.068	1.00	74.64	A
ATOM	468	C	TYR	A	68	-22.659	27.595	74.054	1.00	96.00	A
ATOM	469	O	TYR	A	68	-22.832	28.708	74.556	1.00	96.00	A
ATOM	470	N	GLU	A	69	-22.390	26.507	74.767	1.00	113.97	A
ATOM	471	CA	GLU	A	69	-22.289	26.532	76.218	1.00	113.97	A
ATOM	472	CB	GLU	A	69	-22.451	25.111	76.756	1.00	132.01	A
ATOM	473	CG	GLU	A	69	-23.712	24.425	76.252	1.00	132.01	A
ATOM	474	CD	GLU	A	69	-23.775	22.957	76.623	1.00	132.01	A
ATOM	475	OE1	GLU	A	69	-22.836	22.214	76.268	1.00	132.01	A
ATOM	476	OE2	GLU	A	69	-24.766	22.546	77.263	1.00	132.01	A
ATOM	477	C	GLU	A	69	-20.970	27.130	76.693	1.00	113.97	A
ATOM	478	O	GLU	A	69	-20.547	26.902	77.825	1.00	113.97	A
ATOM	479	N	GLY	A	70	-20.330	27.900	75.819	1.00	103.38	A
ATOM	480	CA	GLY	A	70	-19.066	28.527	76.163	1.00	103.38	A
ATOM	481	C	GLY	A	70	-19.118	30.039	76.041	1.00	103.38	A
ATOM	482	O	GLY	A	70	-20.160	30.612	75.717	1.00	103.38	A
ATOM	483	N	GLU	A	71	-17.989	30.691	76.301	1.00	97.46	A
ATOM	484	CA	GLU	A	71	-17.910	32.144	76.220	1.00	97.46	A
ATOM	485	CB	GLU	A	71	-16.650	32.646	76.933	1.00	122.18	A
ATOM	486	CG	GLU	A	71	-15.407	31.759	76.786	1.00	122.18	A
ATOM	487	CD	GLU	A	71	-15.064	31.412	75.344	1.00	122.18	A
ATOM	488	OE1	GLU	A	71	-15.702	30.496	74.782	1.00	122.18	A
ATOM	489	OE2	GLU	A	71	-14.158	32.055	74.773	1.00	122.18	A
ATOM	490	C	GLU	A	71	-17.920	32.650	74.782	1.00	97.46	A
ATOM	491	O	GLU	A	71	-17.435	31.976	73.873	1.00	97.46	A
ATOM	492	N	PHE	A	72	-18.477	33.842	74.581	1.00	79.72	A
ATOM	493	CA	PHE	A	72	-18.537	34.443	73.250	1.00	79.72	A
ATOM	494	CB	PHE	A	72	-19.192	33.470	72.255	1.00	65.28	A
ATOM	495	CG	PHE	A	72	-20.676	33.303	72.442	1.00	65.28	A
ATOM	496	CD1	PHE	A	72	-21.566	34.245	71.935	1.00	65.28	A
ATOM	497	CD2	PHE	A	72	-21.183	32.196	73.115	1.00	65.28	A
ATOM	498	CE1	PHE	A	72	-22.943	34.084	72.092	1.00	65.28	A
ATOM	499	CE2	PHE	A	72	-22.558	32.024	73.280	1.00	65.28	A
ATOM	500	CZ	PHE	A	72	-23.439	32.969	72.767	1.00	65.28	A
ATOM	501	C	PHE	A	72	-19.297	35.770	73.246	1.00	79.72	A
ATOM	502	O	PHE	A	72	-20.227	35.973	74.029	1.00	79.72	A
ATOM	503	N	ILE	A	73	-18.895	36.670	72.357	1.00	131.12	A
ATOM	504	CA	ILE	A	73	-19.556	37.958	72.248	1.00	131.12	A
ATOM	505	CB	ILE	A	73	-18.587	39.128	72.494	1.00	107.34	A
ATOM	506	CG2	ILE	A	73	-17.337	38.967	71.644	1.00	107.34	A
ATOM	507	CG1	ILE	A	73	-19.303	40.444	72.182	1.00	107.34	A
ATOM	508	CD1	ILE	A	73	-18.441	41.665	72.295	1.00	107.34	A
ATOM	509	C	ILE	A	73	-20.168	38.133	70.865	1.00	131.12	A
ATOM	510	O	ILE	A	73	-19.466	38.102	69.854	1.00	131.12	A
ATOM	511	N	PRO	A	74	-21.494	38.312	70.803	1.00	110.61	A
ATOM	512	CD	PRO	A	74	-22.468	38.336	71.909	1.00	106.24	A
ATOM	513	CA	PRO	A	74	-22.162	38.492	69.514	1.00	110.61	A
ATOM	514	CB	PRO	A	74	-23.640	38.395	69.879	1.00	106.24	A
ATOM	515	CG	PRO	A	74	-23.672	38.979	71.260	1.00	106.24	A
ATOM	516	C	PRO	A	74	-21.797	39.842	68.912	1.00	110.61	A
ATOM	517	O	PRO	A	74	-22.059	40.884	69.510	1.00	110.61	A

FIGURE 25 CON'T

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ATOM    518  N   GLU A  75     -21.181  39.817  67.736  1.00 87.29      A
ATOM    519  CA  GLU A  75     -20.785  41.044  67.054  1.00 87.29      A
ATOM    520  CB  GLU A  75     -19.602  40.775  66.120  1.00 79.91      A
ATOM    521  CG  GLU A  75     -18.334  40.329  66.830  1.00 79.91      A
ATOM    522  CD  GLU A  75     -17.793  41.382  67.777  1.00 79.91      A
ATOM    523  OE1 GLU A  75     -16.732  41.139  68.391  1.00 79.91      A
ATOM    524  OE2 GLU A  75     -18.425  42.452  67.906  1.00 79.91      A
ATOM    525  C   GLU A  75     -21.952  41.616  66.257  1.00 87.29      A
ATOM    526  O   GLU A  75     -21.756  42.335  65.275  1.00 87.29      A
ATOM    527  N   GLY A  76     -23.166  41.285  66.687  1.00123.51      A
ATOM    528  CA  GLY A  76     -24.353  41.777  66.013  1.00123.51      A
ATOM    529  C   GLY A  76     -24.647  41.069  64.707  1.00123.51      A
ATOM    530  O   GLY A  76     -23.866  40.236  64.247  1.00123.51      A
ATOM    531  N   GLU A  77     -25.783  41.405  64.106  1.00 80.94      A
ATOM    532  CA  GLU A  77     -26.191  40.800  62.849  1.00 80.94      A
ATOM    533  CB  GLU A  77     -27.705  40.910  62.671  1.00 91.89      A
ATOM    534  CG  GLU A  77     -28.511  40.184  63.735  1.00 91.89      A
ATOM    535  CD  GLU A  77     -30.007  40.235  63.471  1.00 91.89      A
ATOM    536  OE1 GLU A  77     -30.777  39.706  64.303  1.00 91.89      A
ATOM    537  OE2 GLU A  77     -30.410  40.803  62.431  1.00 91.89      A
ATOM    538  C   GLU A  77     -25.492  41.462  61.679  1.00 80.94      A
ATOM    539  O   GLU A  77     -24.963  42.566  61.799  1.00 80.94      A

ATOM    540  N   ILE A  78     -25.497  40.777  60.542  1.00 71.96      A
ATOM    541  CA  ILE A  78     -24.861  41.280  59.335  1.00 71.96      A
ATOM    542  CB  ILE A  78     -23.404  40.750  59.232  1.00 94.95      A
ATOM    543  CG2 ILE A  78     -23.412  39.261  58.911  1.00 94.95      A
ATOM    544  CG1 ILE A  78     -22.630  41.506  58.153  1.00 94.95      A
ATOM    545  CD1 ILE A  78     -21.164  41.124  58.085  1.00 94.95      A
ATOM    546  C   ILE A  78     -25.678  40.788  58.142  1.00 71.96      A
ATOM    547  O   ILE A  78     -26.488  39.872  58.274  1.00 71.96      A
ATOM    548  N   SER A  79     -25.482  41.403  56.984  1.00 54.93      A
ATOM    549  CA  SER A  79     -26.202  40.985  55.794  1.00 54.93      A
ATOM    550  CB  SER A  79     -26.898  42.186  55.148  1.00 95.68      A
ATOM    551  OG  SER A  79     -25.958  43.180  54.782  1.00 95.68      A
ATOM    552  C   SER A  79     -25.247  40.330  54.793  1.00 54.93      A
ATOM    553  O   SER A  79     -24.067  40.686  54.708  1.00 54.93      A
ATOM    554  N   PHE A  80     -25.781  39.379  54.033  1.00 53.13      A
ATOM    555  CA  PHE A  80     -25.027  38.632  53.038  1.00 53.13      A
ATOM    556  CB  PHE A  80     -26.002  37.814  52.190  1.00 59.45      A
ATOM    557  CG  PHE A  80     -25.344  36.777  51.327  1.00 59.45      A
ATOM    558  CD1 PHE A  80     -24.815  35.616  51.889  1.00 59.45      A
ATOM    559  CD2 PHE A  80     -25.273  36.946  49.948  1.00 59.45      A
ATOM    560  CE1 PHE A  80     -24.231  34.637  51.086  1.00 59.45      A
ATOM    561  CE2 PHE A  80     -24.688  35.970  49.137  1.00 59.45      A
ATOM    562  CZ  PHE A  80     -24.168  34.815  49.708  1.00 59.45      A
ATOM    563  C   PHE A  80     -24.194  39.534  52.134  1.00 53.13      A
ATOM    564  O   PHE A  80     -23.107  39.153  51.686  1.00 53.13      A
ATOM    565  N   SER A  81     -24.705  40.733  51.870  1.00 50.44      A
ATOM    566  CA  SER A  81     -24.022  41.692  51.002  1.00 50.44      A
ATOM    567  CB  SER A  81     -24.933  42.895  50.733  1.00 64.56      A
ATOM    568  OG  SER A  81     -25.289  43.543  51.947  1.00 64.56      A
ATOM    569  C   SER A  81     -22.696  42.197  51.553  1.00 50.44      A
ATOM    570  O   SER A  81     -21.824  42.639  50.797  1.00 50.44      A
ATOM    571  N   GLU A  82     -22.542  42.139  52.869  1.00 66.85      A
ATOM    572  CA  GLU A  82     -21.321  42.627  53.497  1.00 66.85      A
ATOM    573  CB  GLU A  82     -21.650  43.141  54.900  1.00 83.28      A
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FIGURE 25 CON'T

ATOM	574	CG	GLU	A	82	-22.525	44.394	54.870	1.00	83.28	A
ATOM	575	CD	GLU	A	82	-23.218	44.684	56.189	1.00	83.28	A
ATOM	576	OE1	GLU	A	82	-24.087	43.882	56.598	1.00	83.28	A
ATOM	577	OE2	GLU	A	82	-22.894	45.717	56.815	1.00	83.28	A
ATOM	578	C	GLU	A	82	-20.178	41.609	53.540	1.00	66.85	A
ATOM	579	O	GLU	A	82	-19.022	41.982	53.731	1.00	66.85	A
ATOM	580	N	LEU	A	83	-20.492	40.330	53.345	1.00	56.62	A
ATOM	581	CA	LEU	A	83	-19.459	39.300	53.358	1.00	56.62	A
ATOM	582	CB	LEU	A	83	-20.093	37.912	53.501	1.00	52.40	A
ATOM	583	CG	LEU	A	83	-20.801	37.640	54.828	1.00	52.40	A
ATOM	584	CD1	LEU	A	83	-21.641	36.383	54.724	1.00	52.40	A
ATOM	585	CD2	LEU	A	83	-19.766	37.523	55.931	1.00	52.40	A
ATOM	586	C	LEU	A	83	-18.647	39.357	52.070	1.00	56.62	A
ATOM	587	O	LEU	A	83	-19.192	39.626	50.995	1.00	56.62	A
ATOM	588	N	ARG	A	84	-17.342	39.125	52.173	1.00	53.39	A
ATOM	589	CA	ARG	A	84	-16.496	39.126	50.988	1.00	53.39	A
ATOM	590	CB	ARG	A	84	-15.017	39.007	51.380	1.00	91.29	A
ATOM	591	CG	ARG	A	84	-14.064	39.372	50.250	1.00	91.29	A
ATOM	592	CD	ARG	A	84	-12.663	39.752	50.740	1.00	91.29	A
ATOM	593	NE	ARG	A	84	-11.862	38.615	51.197	1.00	91.29	A
ATOM	594	CZ	ARG	A	84	-11.893	38.111	52.427	1.00	91.29	A
ATOM	595	NH1	ARG	A	84	-12.691	38.639	53.346	1.00	91.29	A
ATOM	596	NH2	ARG	A	84	-11.118	37.081	52.743	1.00	91.29	A
ATOM	597	C	ARG	A	84	-16.955	37.915	50.172	1.00	53.39	A
ATOM	598	O	ARG	A	84	-17.531	36.981	50.723	1.00	53.39	A
ATOM	599	N	ASN	A	85	-16.717	37.937	48.867	1.00	57.59	A
ATOM	600	CA	ASN	A	85	-17.153	36.853	47.992	1.00	57.59	A
ATOM	601	CB	ASN	A	85	-16.558	37.052	46.603	1.00	68.01	A
ATOM	602	CG	ASN	A	85	-17.033	38.333	45.957	1.00	68.01	A
ATOM	603	OD1	ASN	A	85	-18.185	38.734	46.129	1.00	68.01	A
ATOM	604	ND2	ASN	A	85	-16.155	38.979	45.202	1.00	68.01	A
ATOM	605	C	ASN	A	85	-16.853	35.443	48.495	1.00	57.59	A
ATOM	606	O	ASN	A	85	-17.744	34.586	48.536	1.00	57.59	A
ATOM	607	N	ASP	A	86	-15.600	35.217	48.875	1.00	55.76	A
ATOM	608	CA	ASP	A	86	-15.141	33.930	49.383	1.00	55.76	A
ATOM	609	CB	ASP	A	86	-13.758	34.093	50.011	1.00	137.78	A
ATOM	610	CG	ASP	A	86	-12.837	34.954	49.169	1.00	137.78	A
ATOM	611	OD1	ASP	A	86	-12.539	34.564	48.021	1.00	137.78	A
ATOM	612	OD2	ASP	A	86	-12.415	36.025	49.655	1.00	137.78	A
ATOM	613	C	ASP	A	86	-16.105	33.384	50.422	1.00	55.76	A
ATOM	614	O	ASP	A	86	-16.581	32.258	50.310	1.00	55.76	A
ATOM	615	N	TYR	A	87	-16.401	34.193	51.433	1.00	48.09	A
ATOM	616	CA	TYR	A	87	-17.301	33.773	52.502	1.00	48.09	A
ATOM	617	CB	TYR	A	87	-17.201	34.751	53.673	1.00	85.93	A
ATOM	618	CG	TYR	A	87	-15.788	34.829	54.202	1.00	85.93	A
ATOM	619	CD1	TYR	A	87	-15.143	33.686	54.677	1.00	85.93	A
ATOM	620	CE1	TYR	A	87	-13.813	33.724	55.088	1.00	85.93	A
ATOM	621	CD2	TYR	A	87	-15.068	36.021	54.162	1.00	85.93	A
ATOM	622	CE2	TYR	A	87	-13.735	36.071	54.574	1.00	85.93	A
ATOM	623	CZ	TYR	A	87	-13.115	34.917	55.033	1.00	85.93	A
ATOM	624	OH	TYR	A	87	-11.794	34.949	55.420	1.00	85.93	A
ATOM	625	C	TYR	A	87	-18.740	33.620	52.034	1.00	48.09	A
ATOM	626	O	TYR	A	87	-19.474	32.761	52.541	1.00	48.09	A
ATOM	627	N	GLN	A	88	-19.147	34.440	51.063	1.00	44.08	A
ATOM	628	CA	GLN	A	88	-20.513	34.337	50.540	1.00	44.08	A
ATOM	629	CB	GLN	A	88	-20.767	35.371	49.431	1.00	54.63	A
ATOM	630	CG	GLN	A	88	-20.763	36.823	49.883	1.00	54.63	A

ATOM	631	CD	GLN	A	88	-21.411	37.755	48.863	1.00	54.63	A
ATOM	632	OE1	GLN	A	88	-21.115	37.694	47.674	1.00	54.63	A
ATOM	633	NE2	GLN	A	88	-22.296	38.626	49.335	1.00	54.63	A
ATOM	634	C	GLN	A	88	-20.681	32.928	49.966	1.00	44.08	A
ATOM	635	O	GLN	A	88	-21.627	32.229	50.290	1.00	44.08	A
ATOM	636	N	SER	A	89	-19.733	32.524	49.122	1.00	48.72	A
ATOM	637	CA	SER	A	89	-19.754	31.209	48.494	1.00	48.72	A
ATOM	638	CB	SER	A	89	-18.612	31.098	47.491	1.00	56.82	A
ATOM	639	OG	SER	A	89	-18.808	31.996	46.409	1.00	56.82	A
ATOM	640	C	SER	A	89	-19.658	30.090	49.528	1.00	48.72	A
ATOM	641	O	SER	A	89	-20.340	29.067	49.419	1.00	48.72	A
ATOM	642	N	LYS	A	90	-18.816	30.287	50.537	1.00	50.16	A
ATOM	643	CA	LYS	A	90	-18.669	29.292	51.588	1.00	50.16	A
ATOM	644	CB	LYS	A	90	-17.549	29.686	52.554	1.00	67.64	A
ATOM	645	CG	LYS	A	90	-16.155	29.471	51.999	1.00	67.64	A
ATOM	646	CD	LYS	A	90	-15.095	29.962	52.966	1.00	67.64	A
ATOM	647	CE	LYS	A	90	-13.702	29.668	52.446	1.00	67.64	A
ATOM	648	NZ	LYS	A	90	-12.660	30.310	53.293	1.00	67.64	A
ATOM	649	C	LYS	A	90	-19.973	29.144	52.343	1.00	50.16	A
ATOM	650	O	LYS	A	90	-20.401	28.027	52.641	1.00	50.16	A
ATOM	651	N	LEU	A	91	-20.617	30.267	52.649	1.00	45.26	A
ATOM	652	CA	LEU	A	91	-21.879	30.218	53.369	1.00	45.26	A
ATOM	653	CB	LEU	A	91	-22.335	31.632	53.735	1.00	57.37	A
ATOM	654	CG	LEU	A	91	-23.594	31.719	54.610	1.00	57.37	A
ATOM	655	CD1	LEU	A	91	-23.430	30.848	55.854	1.00	57.37	A
ATOM	656	CD2	LEU	A	91	-23.846	33.173	54.999	1.00	57.37	A
ATOM	657	C	LEU	A	91	-22.950	29.506	52.533	1.00	45.26	A
ATOM	658	O	LEU	A	91	-23.776	28.769	53.074	1.00	45.26	A
ATOM	659	N	VAL	A	92	-22.927	29.714	51.217	1.00	42.08	A
ATOM	660	CA	VAL	A	92	-23.894	29.072	50.322	1.00	42.08	A
ATOM	661	CB	VAL	A	92	-23.832	29.683	48.888	1.00	46.56	A
ATOM	662	CG1	VAL	A	92	-24.704	28.879	47.931	1.00	46.56	A
ATOM	663	CG2	VAL	A	92	-24.298	31.134	48.921	1.00	46.56	A
ATOM	664	C	VAL	A	92	-23.628	27.567	50.254	1.00	42.08	A
ATOM	665	O	VAL	A	92	-24.561	26.757	50.226	1.00	42.08	A
ATOM	666	N	LEU	A	93	-22.354	27.190	50.235	1.00	48.30	A
ATOM	667	CA	LEU	A	93	-22.000	25.775	50.211	1.00	48.30	A
ATOM	668	CB	LEU	A	93	-20.479	25.603	50.264	1.00	40.14	A
ATOM	669	CG	LEU	A	93	-19.956	24.161	50.241	1.00	40.14	A
ATOM	670	CD1	LEU	A	93	-20.456	23.449	48.998	1.00	40.14	A
ATOM	671	CD2	LEU	A	93	-18.417	24.163	50.265	1.00	40.14	A
ATOM	672	C	LEU	A	93	-22.652	25.106	51.424	1.00	48.30	A
ATOM	673	O	LEU	A	93	-23.301	24.061	51.297	1.00	48.30	A
ATOM	674	N	ARG	A	94	-22.493	25.718	52.598	1.00	49.80	A
ATOM	675	CA	ARG	A	94	-23.095	25.183	53.822	1.00	49.80	A
ATOM	676	CB	ARG	A	94	-22.714	26.037	55.036	1.00	56.97	A
ATOM	677	CG	ARG	A	94	-23.425	25.620	56.318	1.00	56.97	A
ATOM	678	CD	ARG	A	94	-22.934	24.260	56.798	1.00	56.97	A
ATOM	679	NE	ARG	A	94	-23.634	23.785	57.990	1.00	56.97	A
ATOM	680	CZ	ARG	A	94	-24.781	23.110	57.977	1.00	56.97	A
ATOM	681	NH1	ARG	A	94	-25.377	22.822	56.827	1.00	56.97	A
ATOM	682	NH2	ARG	A	94	-25.325	22.706	59.119	1.00	56.97	A
ATOM	683	C	ARG	A	94	-24.620	25.131	53.710	1.00	49.80	A
ATOM	684	O	ARG	A	94	-25.248	24.167	54.155	1.00	49.80	A
ATOM	685	N	LEU	A	95	-25.217	26.166	53.119	1.00	58.97	A
ATOM	686	CA	LEU	A	95	-26.672	26.204	52.958	1.00	58.97	A

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ATOM    687  CB  LEU A  95     -27.128  27.587  52.468  1.00 59.80      A
ATOM    688  CG  LEU A  95     -27.061  28.699  53.525  1.00 59.80      A
ATOM    689  CD1 LEU A  95     -27.396  30.043  52.905  1.00 59.80      A
ATOM    690  CD2 LEU A  95     -28.026  28.375  54.661  1.00 59.80      A
ATOM    691  C   LEU A  95     -27.161  25.116  52.005  1.00 58.97      A
ATOM    692  O   LEU A  95     -28.223  24.530  52.218  1.00 58.97      A
ATOM    693  N   LEU A  96     -26.398  24.848  50.947  1.00 52.25      A
ATOM    694  CA  LEU A  96     -26.777  23.788  50.012  1.00 52.25      A
ATOM    695  CB  LEU A  96     -25.732  23.649  48.893  1.00 39.29      A
ATOM    696  CG  LEU A  96     -25.807  24.714  47.790  1.00 39.29      A
ATOM    697  CD1 LEU A  96     -24.683  24.540  46.806  1.00 39.29      A
ATOM    698  CD2 LEU A  96     -27.155  24.593  47.086  1.00 39.29      A
ATOM    699  C   LEU A  96     -26.894  22.465  50.772  1.00 52.25      A
ATOM    700  O   LEU A  96     -27.829  21.690  50.556  1.00 52.25      A
ATOM    701  N   LYS A  97     -25.942  22.219  51.667  1.00 61.38      A
ATOM    702  CA  LYS A  97     -25.927  20.994  52.462  1.00 61.38      A
ATOM    703  CB  LYS A  97     -24.729  20.994  53.412  1.00 64.44      A
ATOM    704  CG  LYS A  97     -24.551  19.703  54.207  1.00 64.44      A
ATOM    705  CD  LYS A  97     -23.899  18.619  53.361  1.00 64.44      A
ATOM    706  CE  LYS A  97     -23.566  17.382  54.184  1.00 64.44      A
ATOM    707  NZ  LYS A  97     -24.768  16.670  54.680  1.00 64.44      A
ATOM    708  C   LYS A  97     -27.211  20.852  53.275  1.00 61.38      A
ATOM    709  O   LYS A  97     -27.734  19.747  53.434  1.00 61.38      A
ATOM    710  N   GLU A  98     -27.720  21.968  53.791  1.00 62.33      A
ATOM    711  CA  GLU A  98     -28.944  21.932  54.584  1.00 62.33      A
ATOM    712  CB  GLU A  98     -29.188  23.278  55.271  1.00 83.72      A
ATOM    713  CG  GLU A  98     -28.308  23.498  56.484  1.00 83.72      A
ATOM    714  CD  GLU A  98     -28.430  22.368  57.498  1.00 83.72      A
ATOM    715  OE1 GLU A  98     -29.536  22.178  58.048  1.00 83.72      A
ATOM    716  OE2 GLU A  98     -27.422  21.667  57.740  1.00 83.72      A
ATOM    717  C   GLU A  98     -30.163  21.539  53.767  1.00 62.33      A
ATOM    718  O   GLU A  98     -31.200  21.186  54.327  1.00 62.33      A
ATOM    719  N   ASN A  99     -30.043  21.599  52.445  1.00 61.59      A
ATOM    720  CA  ASN A  99     -31.153  21.224  51.589  1.00 61.59      A
ATOM    721  CB  ASN A  99     -31.361  22.255  50.480  1.00 72.80      A
ATOM    722  CG  ASN A  99     -31.899  23.573  51.007  1.00 72.80      A
ATOM    723  OD1 ASN A  99     -31.174  24.347  51.636  1.00 72.80      A
ATOM    724  ND2 ASN A  99     -33.182  23.826  50.765  1.00 72.80      A
ATOM    725  C   ASN A  99     -30.902  19.857  50.983  1.00 61.59      A
ATOM    726  O   ASN A  99     -31.506  19.500  49.972  1.00 61.59      A
ATOM    727  N   GLY A 100     -30.002  19.100  51.607  1.00 63.74      A
ATOM    728  CA  GLY A 100     -29.684  17.768  51.126  1.00 63.74      A
ATOM    729  C   GLY A 100     -28.749  17.717  49.932  1.00 63.74      A
ATOM    730  O   GLY A 100     -28.641  16.687  49.269  1.00 63.74      A
ATOM    731  N   ILE A 101     -28.071  18.821  49.642  1.00 49.44      A
ATOM    732  CA  ILE A 101     -27.148  18.844  48.515  1.00 49.44      A
ATOM    733  CB  ILE A 101     -27.453  20.023  47.575  1.00 51.42      A
ATOM    734  CG2 ILE A 101     -26.437  20.066  46.432  1.00 51.42      A
ATOM    735  CG1 ILE A 101     -28.873  19.871  47.022  1.00 51.42      A
ATOM    736  CD1 ILE A 101     -29.328  21.045  46.203  1.00 51.42      A
ATOM    737  C   ILE A 101     -25.722  18.951  49.035  1.00 49.44      A
ATOM    738  O   ILE A 101     -25.212  20.049  49.255  1.00 49.44      A
ATOM    739  N   GLY A 102     -25.097  17.795  49.245  1.00 43.56      A
ATOM    740  CA  GLY A 102     -23.734  17.758  49.744  1.00 43.56      A
ATOM    741  C   GLY A 102     -22.955  16.629  49.100  1.00 43.56      A
ATOM    742  O   GLY A 102     -23.513  15.823  48.349  1.00 43.56      A
ATOM    743  N   GLU A 103     -21.665  16.560  49.391  1.00 42.81      A
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ATOM    744  CA  GLU A 103     -20.827  15.517  48.819  1.00 42.81      A
ATOM    745  CB  GLU A 103     -19.385  15.702  49.282  1.00 48.36      A
ATOM    746  CG  GLU A 103     -18.764  16.951  48.688  1.00 48.36      A
ATOM    747  CD  GLU A 103     -17.347  17.165  49.132  1.00 48.36      A
ATOM    748  OE1 GLU A 103     -16.671  18.048  48.569  1.00 48.36      A
ATOM    749  OE2 GLU A 103     -16.905  16.451  50.050  1.00 48.36      A
ATOM    750  C   GLU A 103     -21.321  14.123  49.161  1.00 42.81      A
ATOM    751  O   GLU A 103     -21.320  13.234  48.311  1.00 42.81      A
ATOM    752  N   TYR A 104     -21.751  13.935  50.404  1.00 45.75      A
ATOM    753  CA  TYR A 104     -22.253  12.642  50.838  1.00 45.75      A
ATOM    754  CB  TYR A 104     -22.697  12.707  52.300  1.00 64.47      A
ATOM    755  CG  TYR A 104     -23.400  11.453  52.767  1.00 64.47      A
ATOM    756  CD1 TYR A 104     -22.714  10.245  52.870  1.00 64.47      A
ATOM    757  CE1 TYR A 104     -23.357   9.083  53.292  1.00 64.47      A
ATOM    758  CD2 TYR A 104     -24.754  11.472  53.097  1.00 64.47      A
ATOM    759  CE2 TYR A 104     -25.409  10.317  53.522  1.00 64.47      A
ATOM    760  CZ  TYR A 104     -24.704   9.124  53.618  1.00 64.47      A
ATOM    761  OH  TYR A 104     -25.341   7.977  54.049  1.00 64.47      A
ATOM    762  C   TYR A 104     -23.431  12.202  49.972  1.00 45.75      A
ATOM    763  O   TYR A 104     -23.380  11.156  49.327  1.00 45.75      A
ATOM    764  N   GLU A 105     -24.490  13.007  49.955  1.00 43.71      A
ATOM    765  CA  GLU A 105     -25.683  12.683  49.172  1.00 43.71      A
ATOM    766  CB  GLU A 105     -26.764  13.751  49.376  1.00 62.74      A
ATOM    767  CG  GLU A 105     -27.287  13.911  50.803  1.00 62.74      A
ATOM    768  CD  GLU A 105     -26.311  14.619  51.723  1.00 62.74      A
ATOM    769  OE1 GLU A 105     -25.458  15.386  51.225  1.00 62.74      A
ATOM    770  OE2 GLU A 105     -26.407  14.421  52.952  1.00 62.74      A
ATOM    771  C   GLU A 105     -25.431  12.526  47.662  1.00 43.71      A
ATOM    772  O   GLU A 105     -25.856  11.544  47.064  1.00 43.71      A
ATOM    773  N   LEU A 106     -24.754  13.490  47.040  1.00 39.82      A
ATOM    774  CA  LEU A 106     -24.504  13.402  45.606  1.00 39.82      A
ATOM    775  CB  LEU A 106     -24.109  14.779  45.042  1.00 40.67      A
ATOM    776  CG  LEU A 106     -25.330  15.671  44.722  1.00 40.67      A
ATOM    777  CD1 LEU A 106     -26.094  16.030  45.998  1.00 40.67      A
ATOM    778  CD2 LEU A 106     -24.872  16.930  44.023  1.00 40.67      A
ATOM    779  C   LEU A 106     -23.489  12.325  45.204  1.00 39.82      A
ATOM    780  O   LEU A 106     -23.542  11.822  44.082  1.00 39.82      A
ATOM    781  N   SER A 107     -22.570  11.966  46.103  1.00 38.34      A
ATOM    782  CA  SER A 107     -21.611  10.905  45.794  1.00 38.34      A
ATOM    783  CB  SER A 107     -20.526  10.800  46.870  1.00 39.34      A
ATOM    784  OG  SER A 107     -19.582  11.852  46.752  1.00 38.34      A
ATOM    785  C   SER A 107     -22.385   9.589  45.706  1.00 38.34      A
ATOM    786  O   SER A 107     -22.087   8.730  44.872  1.00 38.34      A
ATOM    787  N   LYS A 108     -23.388   9.436  46.568  1.00 46.95      A
ATOM    788  CA  LYS A 108     -24.212   8.231  46.549  1.00 46.95      A
ATOM    789  CB  LYS A 108     -25.175   8.218  47.740  1.00 70.68      A
ATOM    790  CG  LYS A 108     -24.480   7.977  49.075  1.00 70.68      A
ATOM    791  CD  LYS A 108     -25.396   8.254  50.258  1.00 70.68      A
ATOM    792  CE  LYS A 108     -26.610   7.350  50.247  1.00 70.68      A
ATOM    793  NZ  LYS A 108     -27.445   7.570  51.455  1.00 70.68      A
ATOM    794  C   LYS A 108     -24.990   8.184  45.235  1.00 46.95      A
ATOM    795  O   LYS A 108     -25.078   7.141  44.600  1.00 46.95      A

ATOM    796  N   LEU A 109     -25.549   9.319  44.825  1.00 42.18      A
ATOM    797  CA  LEU A 109     -26.291   9.376  43.575  1.00 42.18      A
ATOM    798  CB  LEU A 109     -26.873  10.783  43.358  1.00 40.49      A
ATOM    799  CG  LEU A 109     -27.945  11.260  44.354  1.00 40.49      A
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FIGURE 25 CON'T

ATOM	800	CD1	LEU	A	109	-28.387	12.689	44.012	1.00 40.49	A
ATOM	801	CD2	LEU	A	109	-29.150	10.316	44.331	1.00 40.49	A
ATOM	802	C	LEU	A	109	-25.373	8.983	42.410	1.00 42.18	A
ATOM	803	O	LEU	A	109	-25.772	8.217	41.539	1.00 42.18	A
ATOM	804	N	LEU	A	110	-24.146	9.499	42.395	1.00 37.22	A
ATOM	805	CA	LEU	A	110	-23.194	9.163	41.329	1.00 37.22	A
ATOM	806	CB	LEU	A	110	-21.843	9.869	41.557	1.00 28.86	A
ATOM	807	CG	LEU	A	110	-20.639	9.415	40.701	1.00 28.86	A
ATOM	808	CD1	LEU	A	110	-20.876	9.791	39.218	1.00 28.86	A
ATOM	809	CD2	LEU	A	110	-19.329	10.081	41.214	1.00 28.86	A
ATOM	810	C	LEU	A	110	-22.943	7.658	41.215	1.00 37.22	A
ATOM	811	O	LEU	A	110	-22.899	7.101	40.101	1.00 37.22	A
ATOM	812	N	ARG	A	111	-22.761	7.001	42.356	1.00 45.48	A
ATOM	813	CA	ARG	A	111	-22.495	5.569	42.353	1.00 45.48	A
ATOM	814	CB	ARG	A	111	-21.988	5.111	43.730	1.00 39.33	A
ATOM	815	CG	ARG	A	111	-20.594	5.692	44.031	1.00 39.33	A
ATOM	816	CD	ARG	A	111	-19.960	5.096	45.270	1.00 39.33	A
ATOM	817	NE	ARG	A	111	-20.584	5.586	46.496	1.00 39.33	A
ATOM	818	CZ	ARG	A	111	-20.157	6.633	47.196	1.00 39.33	A
ATOM	819	NH1	ARG	A	111	-19.089	7.316	46.794	1.00 39.33	A
ATOM	820	NH2	ARG	A	111	-20.799	6.990	48.305	1.00 39.33	A
ATOM	821	C	ARG	A	111	-23.685	4.737	41.891	1.00 45.48	A
ATOM	822	O	ARG	A	111	-23.585	3.516	41.753	1.00 45.48	A
ATOM	823	N	LYS	A	112	-24.808	5.397	41.629	1.00 49.69	A
ATOM	824	CA	LYS	A	112	-25.963	4.676	41.122	1.00 49.69	A
ATOM	825	CB	LYS	A	112	-27.249	5.481	41.321	1.00 66.26	A
ATOM	826	CG	LYS	A	112	-27.793	5.461	42.733	1.00 66.26	A
ATOM	827	CD	LYS	A	112	-29.187	6.068	42.771	1.00 66.26	A
ATOM	828	CE	LYS	A	112	-29.856	5.845	44.120	1.00 66.26	A
ATOM	829	NZ	LYS	A	112	-31.276	6.297	44.113	1.00 66.26	A
ATOM	830	C	LYS	A	112	-25.729	4.455	39.629	1.00 49.69	A
ATOM	831	O	LYS	A	112	-26.286	3.531	39.032	1.00 49.69	A
ATOM	832	N	PHE	A	113	-24.881	5.301	39.045	1.00 44.64	A
ATOM	833	CA	PHE	A	113	-24.569	5.248	37.614	1.00 44.64	A
ATOM	834	CB	PHE	A	113	-24.845	6.617	36.996	1.00 42.87	A
ATOM	835	CG	PHE	A	113	-26.215	7.152	37.323	1.00 42.87	A
ATOM	836	CD1	PHE	A	113	-27.331	6.729	36.607	1.00 42.87	A
ATOM	837	CD2	PHE	A	113	-26.397	8.034	38.386	1.00 42.87	A
ATOM	838	CE1	PHE	A	113	-28.608	7.171	36.948	1.00 42.87	A
ATOM	839	CE2	PHE	A	113	-27.675	8.483	38.735	1.00 42.87	A
ATOM	840	CZ	PHE	A	113	-28.782	8.047	38.014	1.00 42.87	A
ATOM	841	C	PHE	A	113	-23.133	4.827	37.313	1.00 44.64	A
ATOM	842	O	PHE	A	113	-22.881	4.157	36.309	1.00 44.64	A
ATOM	843	N	ARG	A	114	-22.198	5.243	38.169	1.00 42.32	A
ATOM	844	CA	ARG	A	114	-20.784	4.899	38.022	1.00 42.32	A
ATOM	845	CB	ARG	A	114	-19.933	6.167	37.868	1.00 50.54	A
ATOM	846	CG	ARG	A	114	-18.470	5.926	37.474	1.00 50.54	A
ATOM	847	CD	ARG	A	114	-18.357	5.175	36.149	1.00 50.54	A
ATOM	848	NE	ARG	A	114	-17.008	5.231	35.590	1.00 50.54	A
ATOM	849	CZ	ARG	A	114	-16.596	4.539	34.529	1.00 50.54	A
ATOM	850	NH1	ARG	A	114	-17.430	3.723	33.896	1.00 50.54	A
ATOM	851	NH2	ARG	A	114	-15.344	4.648	34.106	1.00 50.54	A
ATOM	852	C	ARG	A	114	-20.428	4.167	39.316	1.00 42.32	A
ATOM	853	O	ARG	A	114	-20.106	4.785	40.339	1.00 42.32	A
ATOM	854	N	LYS	A	115	-20.496	2.844	39.260	1.00 44.60	A
ATOM	855	CA	LYS	A	115	-20.248	2.008	40.433	1.00 44.60	A
ATOM	856	CB	LYS	A	115	-20.946	0.657	40.255	1.00 77.56	A

ATOM	857	CG	LYS	A	115	-22.445	0.743	40.062	1.00	77.56	A
ATOM	858	CD	LYS	A	115	-23.035	-0.639	39.853	1.00	77.56	A
ATOM	859	CE	LYS	A	115	-24.543	-0.582	39.674	1.00	77.56	A
ATOM	860	NZ	LYS	A	115	-25.133	-1.952	39.542	1.00	77.56	A
ATOM	861	C	LYS	A	115	-18.795	1.747	40.795	1.00	44.60	A
ATOM	862	O	LYS	A	115	-17.912	1.822	39.954	1.00	44.60	A
ATOM	863	N	PRO	A	116	-18.534	1.449	42.076	1.00	45.82	A
ATOM	864	CD	PRO	A	116	-19.441	1.560	43.227	1.00	41.36	A
ATOM	865	CA	PRO	A	116	-17.172	1.161	42.521	1.00	45.82	A
ATOM	866	CB	PRO	A	116	-17.343	0.883	44.013	1.00	41.36	A
ATOM	867	CG	PRO	A	116	-18.457	1.773	44.387	1.00	41.36	A
ATOM	868	C	PRO	A	116	-16.751	-0.094	41.772	1.00	45.82	A
ATOM	869	O	PRO	A	116	-17.578	-0.970	41.504	1.00	45.82	A
ATOM	870	N	LYS	A	117	-15.474	-0.194	41.442	1.00	44.22	A
ATOM	871	CA	LYS	A	117	-15.002	-1.361	40.724	1.00	44.22	A
ATOM	872	CB	LYS	A	117	-14.766	-1.003	39.258	1.00	53.13	A
ATOM	873	CG	LYS	A	117	-14.467	-2.185	38.357	1.00	53.13	A
ATOM	874	CD	LYS	A	117	-14.588	-1.775	36.896	1.00	53.13	A
ATOM	875	CE	LYS	A	117	-14.312	-2.934	35.946	1.00	53.13	A
ATOM	876	NZ	LYS	A	117	-14.623	-2.553	34.526	1.00	53.13	A
ATOM	877	C	LYS	A	117	-13.712	-1.820	41.380	1.00	44.22	A
ATOM	878	O	LYS	A	117	-12.877	-1.004	41.766	1.00	44.22	A
ATOM	879	N	THR	A	118	-13.553	-3.131	41.509	1.00	52.99	A
ATOM	880	CA	THR	A	118	-12.363	-3.672	42.135	1.00	52.99	A
ATOM	881	CB	THR	A	118	-12.730	-4.747	43.168	1.00	74.27	A
ATOM	882	OG1	THR	A	118	-13.546	-5.744	42.546	1.00	74.27	A
ATOM	883	CG2	THR	A	118	-13.496	-4.128	44.325	1.00	74.27	A
ATOM	884	C	THR	A	118	-11.394	-4.260	41.130	1.00	52.99	A
ATOM	885	O	THR	A	118	-11.786	-4.960	40.201	1.00	52.99	A
ATOM	886	N	PHE	A	119	-10.123	-3.941	41.319	1.00	43.70	A
ATOM	887	CA	PHE	A	119	-9.043	-4.434	40.469	1.00	43.70	A
ATOM	888	CB	PHE	A	119	-8.372	-3.274	39.714	1.00	50.21	A
ATOM	889	CG	PHE	A	119	-9.294	-2.541	38.763	1.00	50.21	A
ATOM	890	CD1	PHE	A	119	-9.266	-2.811	37.393	1.00	50.21	A
ATOM	891	CD2	PHE	A	119	-10.199	-1.597	39.239	1.00	50.21	A
ATOM	892	CE1	PHE	A	119	-10.137	-2.142	36.508	1.00	50.21	A
ATOM	893	CE2	PHE	A	119	-11.067	-0.931	38.371	1.00	50.21	A
ATOM	894	CZ	PHE	A	119	-11.037	-1.202	37.003	1.00	50.21	A
ATOM	895	C	PHE	A	119	-8.055	-5.046	41.454	1.00	43.70	A
ATOM	896	O	PHE	A	119	-7.467	-4.328	42.280	1.00	43.70	A
ATOM	897	N	GLY	A	120	-7.883	-6.364	41.393	1.00	44.94	A
ATOM	898	CA	GLY	A	120	-6.966	-7.019	42.312	1.00	44.94	A
ATOM	899	C	GLY	A	120	-7.471	-6.796	43.723	1.00	44.94	A
ATOM	900	O	GLY	A	120	-8.652	-7.033	44.002	1.00	44.94	A
ATOM	901	N	ASP	A	121	-6.598	-6.326	44.610	1.00	55.66	A
ATOM	902	CA	ASP	A	121	-6.980	-6.071	45.999	1.00	55.66	A
ATOM	903	CB	ASP	A	121	-5.795	-6.302	46.950	1.00	64.03	A
ATOM	904	CG	ASP	A	121	-5.403	-7.762	47.070	1.00	64.03	A
ATOM	905	OD1	ASP	A	121	-6.305	-8.622	47.160	1.00	64.03	A
ATOM	906	OD2	ASP	A	121	-4.186	-8.043	47.095	1.00	64.03	A
ATOM	907	C	ASP	A	121	-7.467	-4.643	46.214	1.00	55.66	A
ATOM	908	O	ASP	A	121	-7.723	-4.242	47.350	1.00	55.66	A
ATOM	909	N	TYR	A	122	-7.598	-3.874	45.140	1.00	49.08	A
ATOM	910	CA	TYR	A	122	-8.014	-2.485	45.276	1.00	49.08	A
ATOM	911	CB	TYR	A	122	-6.972	-1.577	44.618	1.00	51.10	A
ATOM	912	CG	TYR	A	122	-5.632	-1.582	45.312	1.00	51.10	A
ATOM	913	CD1	TYR	A	122	-5.347	-0.674	46.343	1.00	51.10	A

ATOM	914	CE1	TYR	A	122	-4.136	-0.713	47.018	1.00 51.10	A
ATOM	915	CD2	TYR	A	122	-4.665	-2.526	44.977	1.00 51.10	A
ATOM	916	CE2	TYR	A	122	-3.443	-2.577	45.648	1.00 51.10	A
ATOM	917	CZ	TYR	A	122	-3.186	-1.672	46.666	1.00 51.10	A
ATOM	918	OH	TYR	A	122	-1.991	-1.748	47.334	1.00 51.10	A
ATOM	919	C	TYR	A	122	-9.396	-2.162	44.713	1.00 49.08	A
ATOM	920	O	TYR	A	122	-9.815	-2.703	43.694	1.00 49.08	A
ATOM	921	N	LYS	A	123	-10.110	-1.276	45.389	1.00 46.45	A
ATOM	922	CA	LYS	A	123	-11.421	-0.875	44.912	1.00 46.45	A
ATOM	923	CB	LYS	A	123	-12.487	-1.060	45.995	1.00 59.84	A
ATOM	924	CG	LYS	A	123	-13.869	-0.625	45.526	1.00 59.84	A
ATOM	925	CD	LYS	A	123	-14.896	-0.609	46.648	1.00 59.84	A
ATOM	926	CE	LYS	A	123	-15.216	-2.012	47.147	1.00 59.84	A
ATOM	927	NZ	LYS	A	123	-16.267	-1.971	48.202	1.00 59.84	A
ATOM	928	C	LYS	A	123	-11.369	0.597	44.518	1.00 46.45	A
ATOM	929	O	LYS	A	123	-10.870	1.423	45.281	1.00 46.45	A
ATOM	930	N	VAL	A	124	-11.858	0.910	43.322	1.00 43.32	A
ATOM	931	CA	VAL	A	124	-11.918	2.288	42.843	1.00 43.32	A
ATOM	932	CB	VAL	A	124	-11.800	2.382	41.313	1.00 44.39	A
ATOM	933	CG1	VAL	A	124	-11.982	3.837	40.884	1.00 44.39	A
ATOM	934	CG2	VAL	A	124	-10.447	1.857	40.856	1.00 44.39	A
ATOM	935	C	VAL	A	124	-13.290	2.823	43.242	1.00 43.32	A
ATOM	936	O	VAL	A	124	-14.317	2.299	42.812	1.00 43.32	A
ATOM	937	N	ILE	A	125	-13.306	3.874	44.051	1.00 34.73	A
ATOM	938	CA	ILE	A	125	-14.553	4.436	44.530	1.00 34.73	A
ATOM	939	CB	ILE	A	125	-14.541	4.499	46.075	1.00 39.71	A
ATOM	940	CG2	ILE	A	125	-15.887	4.976	46.592	1.00 39.71	A
ATOM	941	CG1	ILE	A	125	-14.182	3.123	46.639	1.00 39.71	A
ATOM	942	CD1	ILE	A	125	-14.110	3.068	48.154	1.00 39.71	A
ATOM	943	C	ILE	A	125	-14.856	5.829	43.986	1.00 34.73	A
ATOM	944	O	ILE	A	125	-14.173	6.798	44.327	1.00 34.73	A
ATOM	945	N	PRO	A	126	-15.877	5.949	43.122	1.00 42.89	A
ATOM	946	CD	PRO	A	126	-16.561	4.868	42.383	1.00 37.78	A
ATOM	947	CA	PRO	A	126	-16.225	7.269	42.572	1.00 42.89	A
ATOM	948	CB	PRO	A	126	-17.132	6.942	41.375	1.00 37.78	A
ATOM	949	CG	PRO	A	126	-16.767	5.492	41.020	1.00 37.78	A
ATOM	950	C	PRO	A	126	-16.993	8.071	43.608	1.00 42.89	A
ATOM	951	O	PRO	A	126	-17.765	7.508	44.396	1.00 42.89	A
ATOM	952	N	SER	A	127	-16.782	9.385	43.611	1.00 41.13	A
ATOM	953	CA	SER	A	127	-17.506	10.268	44.519	1.00 41.13	A
ATOM	954	CB	SER	A	127	-16.859	10.272	45.912	1.00 36.83	A
ATOM	955	OG	SER	A	127	-15.702	11.086	45.931	1.00 36.83	A
ATOM	956	C	SER	A	127	-17.448	11.664	43.898	1.00 41.13	A
ATOM	957	O	SER	A	127	-16.843	11.848	42.842	1.00 41.13	A
ATOM	958	N	VAL	A	128	-18.088	12.642	44.524	1.00 41.04	A
ATOM	959	CA	VAL	A	128	-18.025	13.989	43.985	1.00 41.04	A
ATOM	960	CB	VAL	A	128	-19.399	14.532	43.538	1.00 42.52	A
ATOM	961	CG1	VAL	A	128	-19.995	13.633	42.454	1.00 42.52	A
ATOM	962	CG2	VAL	A	128	-20.325	14.647	44.736	1.00 42.52	A
ATOM	963	C	VAL	A	128	-17.459	14.980	44.978	1.00 41.04	A
ATOM	964	O	VAL	A	128	-17.731	14.923	46.175	1.00 41.04	A
ATOM	965	N	GLU	A	129	-16.672	15.898	44.445	1.00 39.23	A
ATOM	966	CA	GLU	A	129	-16.056	16.966	45.209	1.00 39.23	A
ATOM	967	CB	GLU	A	129	-14.622	17.111	44.716	1.00 59.10	A
ATOM	968	CG	GLU	A	129	-13.759	18.136	45.388	1.00 59.10	A
ATOM	969	CD	GLU	A	129	-12.330	18.002	44.909	1.00 59.10	A

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ATOM	970	OE1	GLU	A	129	-11.606	17.123	45.422	1.00 59.10	A
ATOM	971	OE2	GLU	A	129	-11.938	18.748	43.997	1.00 59.10	A
ATOM	972	C	GLU	A	129	-16.909	18.200	44.858	1.00 39.23	A
ATOM	973	O	GLU	A	129	-17.144	18.476	43.681	1.00 39.23	A
ATOM	974	N	MSE	A	130	-17.379	18.932	45.864	1.00 46.88	A
ATOM	975	CA	MSE	A	130	-18.217	20.100	45.594	1.00 46.88	A
ATOM	976	CB	MSE	A	130	-19.645	19.832	46.076	1.00 52.07	A
ATOM	977	CG	MSE	A	130	-20.450	18.959	45.129	1.00 52.07	A
ATOM	978	SE	MSE	A	130	-21.832	17.956	46.025	1.00 52.07	A
ATOM	979	CE	MSE	A	130	-22.671	19.372	47.043	1.00 52.07	A
ATOM	980	C	MSE	A	130	-17.739	21.425	46.177	1.00 46.88	A
ATOM	981	O	MSE	A	130	-17.205	21.477	47.287	1.00 46.88	A
ATOM	982	N	SER	A	131	-17.954	22.498	45.416	1.00 38.88	A
ATOM	983	CA	SER	A	131	-17.580	23.840	45.846	1.00 38.88	A
ATOM	984	CB	SER	A	131	-16.118	24.140	45.483	1.00 37.16	A
ATOM	985	OG	SER	A	131	-15.933	24.200	44.082	1.00 37.16	A
ATOM	986	C	SER	A	131	-18.517	24.863	45.197	1.00 38.88	A
ATOM	987	O	SER	A	131	-19.308	24.529	44.316	1.00 38.88	A
ATOM	988	N	VAL	A	132	-18.436	26.106	45.653	1.00 43.58	A
ATOM	989	CA	VAL	A	132	-19.269	27.175	45.130	1.00 43.58	A
ATOM	990	CB	VAL	A	132	-20.210	27.731	46.211	1.00 43.96	A
ATOM	991	CG1	VAL	A	132	-20.951	28.969	45.685	1.00 43.96	A
ATOM	992	CG2	VAL	A	132	-21.188	26.656	46.643	1.00 43.96	A
ATOM	993	C	VAL	A	132	-18.406	28.312	44.610	1.00 43.58	A
ATOM	994	O	VAL	A	132	-17.508	28.802	45.307	1.00 43.58	A
ATOM	995	N	ILE	A	133	-18.683	28.717	43.373	1.00 43.62	A
ATOM	996	CA	ILE	A	133	-17.968	29.807	42.732	1.00 43.62	A
ATOM	997	CB	ILE	A	133	-17.324	29.349	41.409	1.00 42.01	A
ATOM	998	CG2	ILE	A	133	-16.682	30.540	40.710	1.00 42.01	A
ATOM	999	CG1	ILE	A	133	-16.247	28.290	41.673	1.00 42.01	A
ATOM	1000	CD1	ILE	A	133	-15.498	27.875	40.405	1.00 42.01	A
ATOM	1001	C	ILE	A	133	-18.945	30.955	42.427	1.00 43.62	A
ATOM	1002	O	ILE	A	133	-20.065	30.730	41.945	1.00 43.62	A
ATOM	1003	N	LYS	A	134	-18.538	32.182	42.730	1.00 47.61	A
ATOM	1004	CA	LYS	A	134	-19.389	33.328	42.429	1.00 47.61	A
ATOM	1005	CB	LYS	A	134	-19.263	34.412	43.504	1.00 46.47	A
ATOM	1006	CG	LYS	A	134	-20.306	35.536	43.371	1.00 46.47	A
ATOM	1007	CD	LYS	A	134	-19.960	36.727	44.246	1.00 46.47	A
ATOM	1008	CE	LYS	A	134	-21.094	37.759	44.307	1.00 46.47	A
ATOM	1009	NZ	LYS	A	134	-20.755	38.892	45.219	1.00 46.47	A
ATOM	1010	C	LYS	A	134	-18.875	33.864	41.097	1.00 47.61	A
ATOM	1011	O	LYS	A	134	-17.729	34.306	41.013	1.00 47.61	A
ATOM	1012	N	HIS	A	135	-19.677	33.791	40.040	1.00 73.70	A
ATOM	1013	CA	HIS	A	135	-19.179	34.309	38.781	1.00 73.70	A
ATOM	1014	CB	HIS	A	135	-20.037	33.868	37.605	1.00 60.65	A
ATOM	1015	CG	HIS	A	135	-19.483	34.299	36.288	1.00 60.65	A
ATOM	1016	CD2	HIS	A	135	-20.090	34.643	35.129	1.00 60.65	A
ATOM	1017	ND1	HIS	A	135	-18.129	34.420	36.065	1.00 60.65	A
ATOM	1018	CE1	HIS	A	135	-17.924	34.821	34.823	1.00 60.65	A
ATOM	1019	NE2	HIS	A	135	-19.098	34.964	34.234	1.00 60.65	A
ATOM	1020	C	HIS	A	135	-19.158	35.824	38.925	1.00 73.70	A
ATOM	1021	O	HIS	A	135	-18.138	36.378	39.334	1.00 73.70	A
ATOM	1022	N	ASP	A	136	-20.241	36.514	38.589	1.00 66.01	A
ATOM	1023	CA	ASP	A	136	-20.230	37.957	38.819	1.00 66.01	A
ATOM	1024	CB	ASP	A	136	-20.599	38.762	37.562	1.00 86.73	A
ATOM	1025	CG	ASP	A	136	-21.682	38.121	36.745	1.00 86.73	A
ATOM	1026	OD1	ASP	A	136	-22.771	37.856	37.297	1.00 86.73	A

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ATOM	1027	OD2	ASP	A	136	-21.442	37.894	35.540	1.00 86.73	A
ATOM	1028	C	ASP	A	136	-21.188	38.229	39.975	1.00 66.01	A
ATOM	1029	O	ASP	A	136	-20.750	38.464	41.099	1.00 66.01	A
ATOM	1030	N	GLU	A	137	-22.488	38.167	39.726	1.00 48.31	A
ATOM	1031	CA	GLU	A	137	-23.454	38.379	40.801	1.00 48.31	A
ATOM	1032	CB	GLU	A	137	-24.469	39.455	40.392	1.00110.10	A
ATOM	1033	CG	GLU	A	137	-25.060	39.267	38.999	1.00110.10	A
ATOM	1034	CD	GLU	A	137	-26.069	40.347	38.631	1.00110.10	A
ATOM	1035	OE1	GLU	A	137	-25.735	41.548	38.746	1.00110.10	A
ATOM	1036	OE2	GLU	A	137	-27.195	39.992	38.218	1.00110.10	A
ATOM	1037	C	GLU	A	137	-24.185	37.078	41.164	1.00 48.31	A
ATOM	1038	O	GLU	A	137	-24.998	37.049	42.083	1.00 48.31	A
ATOM	1039	N	ASP	A	138	-23.873	36.001	40.452	1.00 47.89	A
ATOM	1040	CA	ASP	A	138	-24.520	34.708	40.681	1.00 47.89	A
ATOM	1041	CB	ASP	A	138	-25.025	34.166	39.350	1.00 55.11	A
ATOM	1042	CG	ASP	A	138	-26.057	35.069	38.721	1.00 55.11	A
ATOM	1043	OD1	ASP	A	138	-27.145	35.214	39.315	1.00 55.11	A
ATOM	1044	OD2	ASP	A	138	-25.775	35.640	37.646	1.00 55.11	A
ATOM	1045	C	ASP	A	138	-23.631	33.663	41.353	1.00 47.89	A
ATOM	1046	O	ASP	A	138	-22.409	33.753	41.313	1.00 47.89	A
ATOM	1047	N	PHE	A	139	-24.254	32.674	41.979	1.00 46.35	A
ATOM	1048	CA	PHE	A	139	-23.506	31.611	42.644	1.00 46.35	A
ATOM	1049	CB	PHE	A	139	-23.936	31.494	44.106	1.00 44.51	A
ATOM	1050	CG	PHE	A	139	-23.541	32.678	44.939	1.00 44.51	A
ATOM	1051	CD1	PHE	A	139	-22.281	32.743	45.526	1.00 44.51	A
ATOM	1052	CD2	PHE	A	139	-24.415	33.752	45.100	1.00 44.51	A
ATOM	1053	CE1	PHE	A	139	-21.891	33.863	46.260	1.00 44.51	A
ATOM	1054	CE2	PHE	A	139	-24.038	34.880	45.836	1.00 44.51	A
ATOM	1055	CZ	PHE	A	139	-22.775	34.936	46.415	1.00 44.51	A
ATOM	1056	C	PHE	A	139	-23.726	30.298	41.915	1.00 46.35	A
ATOM	1057	O	PHE	A	139	-24.855	29.954	41.562	1.00 46.35	A
ATOM	1058	N	TYR	A	140	-22.630	29.577	41.693	1.00 41.55	A
ATOM	1059	CA	TYR	A	140	-22.662	28.304	40.992	1.00 41.55	A
ATOM	1060	CB	TYR	A	140	-21.934	28.440	39.657	1.00 47.06	A
ATOM	1061	CG	TYR	A	140	-22.594	29.410	38.703	1.00 47.06	A
ATOM	1062	CD1	TYR	A	140	-23.511	28.964	37.749	1.00 47.06	A
ATOM	1063	CE1	TYR	A	140	-24.139	29.857	36.881	1.00 47.06	A
ATOM	1064	CD2	TYR	A	140	-22.320	30.776	38.768	1.00 47.06	A
ATOM	1065	CE2	TYR	A	140	-22.942	31.677	37.911	1.00 47.06	A
ATOM	1066	CZ	TYR	A	140	-23.851	31.207	36.972	1.00 47.06	A
ATOM	1067	OH	TYR	A	140	-24.487	32.091	36.138	1.00 47.06	A
ATOM	1068	C	TYR	A	140	-22.040	27.159	41.787	1.00 41.55	A
ATOM	1069	O	TYR	A	140	-20.998	27.305	42.438	1.00 41.55	A
ATOM	1070	N	LEU	A	141	-22.696	26.012	41.726	1.00 41.62	A
ATOM	1071	CA	LEU	A	141	-22.220	24.834	42.410	1.00 41.62	A
ATOM	1072	CB	LEU	A	141	-23.396	23.978	42.876	1.00 36.37	A
ATOM	1073	CG	LEU	A	141	-22.993	22.587	43.380	1.00 36.37	A
ATOM	1074	CD1	LEU	A	141	-22.221	22.707	44.680	1.00 36.37	A
ATOM	1075	CD2	LEU	A	141	-24.234	21.738	43.583	1.00 36.37	A
ATOM	1076	C	LEU	A	141	-21.371	24.044	41.427	1.00 41.62	A
ATOM	1077	O	LEU	A	141	-21.819	23.740	40.323	1.00 41.62	A
ATOM	1078	N	VAL	A	142	-20.137	23.743	41.823	1.00 39.96	A
ATOM	1079	CA	VAL	A	142	-19.238	22.960	40.993	1.00 39.96	A
ATOM	1080	CB	VAL	A	142	-17.763	23.401	41.169	1.00 31.71	A
ATOM	1081	CG1	VAL	A	142	-16.862	22.590	40.231	1.00 31.71	A
ATOM	1082	CG2	VAL	A	142	-17.613	24.898	40.886	1.00 31.71	A

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ATOM   1083  C   VAL A 142     -19.371  21.519  41.476  1.00 39.96      A
ATOM   1084  O   VAL A 142     -19.204  21.245  42.672  1.00 39.96      A
ATOM   1085  N   ILE A 143     -19.715  20.609  40.562  1.00 35.84      A
ATOM   1086  CA  ILE A 143     -19.838  19.201  40.900  1.00 35.84      A
ATOM   1087  CB  ILE A 143     -21.208  18.622  40.508  1.00 43.14      A
ATOM   1088  CG2 ILE A 143     -21.312  17.186  40.996  1.00 43.14      A
ATOM   1089  CG1 ILE A 143     -22.332  19.464  41.118  1.00 43.14      A
ATOM   1090  CD1 ILE A 143     -23.726  18.935  40.785  1.00 43.14      A
ATOM   1091  C   ILE A 143     -18.760  18.526  40.084  1.00 35.84      A
ATOM   1092  O   ILE A 143     -18.836  18.476  38.845  1.00 35.84      A
ATOM   1093  N   HIS A 144     -17.756  18.002  40.782  1.00 37.56      A
ATOM   1094  CA  HIS A 144     -16.610  17.384  40.138  1.00 37.56      A
ATOM   1095  CB  HIS A 144     -15.364  18.235  40.458  1.00 36.74      A
ATOM   1096  CG  HIS A 144     -14.069  17.660  39.965  1.00 36.74      A
ATOM   1097  CD2 HIS A 144     -12.882  17.474  40.597  1.00 36.74      A
ATOM   1098  ND1 HIS A 144     -13.888  17.214  38.672  1.00 36.74      A
ATOM   1099  CE1 HIS A 144     -12.649  16.771  38.527  1.00 36.74      A
ATOM   1100  NE2 HIS A 144     -12.017  16.919  39.681  1.00 36.74      A
ATOM   1101  C   HIS A 144     -16.425  15.937  40.565  1.00 37.56      A
ATOM   1102  O   HIS A 144     -16.318  15.619  41.759  1.00 37.56      A
ATOM   1103  N   ILE A 145     -16.387  15.060  39.565  1.00 38.15      A
ATOM   1104  CA  ILE A 145     -16.228  13.630  39.789  1.00 38.15      A
ATOM   1105  CB  ILE A 145     -16.747  12.837  38.570  1.00 37.53      A
ATOM   1106  CG2 ILE A 145     -16.476  11.354  38.765  1.00 37.53      A
ATOM   1107  CG1 ILE A 145     -18.237  13.113  38.370  1.00 37.53      A
ATOM   1108  CD1 ILE A 145     -18.797  12.562  37.054  1.00 37.53      A
ATOM   1109  C   ILE A 145     -14.764  13.253  40.033  1.00 38.15      A
ATOM   1110  O   ILE A 145     -13.888  13.527  39.201  1.00 38.15      A
ATOM   1111  N   ILE A 146     -14.512  12.605  41.169  1.00 35.02      A
ATOM   1112  CA  ILE A 146     -13.165  12.173  41.541  1.00 35.02      A
ATOM   1113  CB  ILE A 146     -12.596  13.013  42.715  1.00 39.08      A
ATOM   1114  CG2 ILE A 146     -12.316  14.451  42.250  1.00 39.08      A
ATOM   1115  CG1 ILE A 146     -13.572  12.980  43.898  1.00 39.08      A
ATOM   1116  CD1 ILE A 146     -13.026  13.632  45.202  1.00 39.08      A
ATOM   1117  C   ILE A 146     -13.192  10.706  41.968  1.00 35.02      A
ATOM   1118  O   ILE A 146     -14.263  10.098  42.046  1.00 35.02      A
ATOM   1119  N   HIS A 147     -12.025  10.143  42.266  1.00 46.27      A
ATOM   1120  CA  HIS A 147     -11.959   8.742  42.665  1.00 46.27      A
ATOM   1121  CB  HIS A 147     -11.571   7.856  41.471  1.00 43.25      A
ATOM   1122  CG  HIS A 147     -12.430   8.050  40.259  1.00 43.25      A
ATOM   1123  CD2 HIS A 147     -13.390   7.266  39.711  1.00 43.25      A
ATOM   1124  ND1 HIS A 147     -12.358   9.178  39.467  1.00 43.25      A
ATOM   1125  CE1 HIS A 147     -13.235   9.078  38.483  1.00 43.25      A
ATOM   1126  NE2 HIS A 147     -13.874   7.927  38.609  1.00 43.25      A
ATOM   1127  C   HIS A 147     -10.969   8.449  43.786  1.00 46.27      A
ATOM   1128  O   HIS A 147      -9.878   9.005  43.830  1.00 46.27      A
ATOM   1129  N   GLN A 148     -11.365   7.557  44.688  1.00 42.59      A
ATOM   1130  CA  GLN A 148     -10.494   7.123  45.761  1.00 42.59      A
ATOM   1131  CB  GLN A 148     -11.223   7.149  47.113  1.00 65.13      A
ATOM   1132  CG  GLN A 148     -11.757   8.519  47.542  1.00 65.13      A
ATOM   1133  CD  GLN A 148     -13.158   8.835  47.000  1.00 65.13      A
ATOM   1134  OE1 GLN A 148     -14.142   8.171  47.346  1.00 65.13      A
ATOM   1135  NE2 GLN A 148     -13.247   9.859  46.154  1.00 65.13      A
ATOM   1136  C   GLN A 148     -10.120   5.678  45.399  1.00 42.59      A
ATOM   1137  O   GLN A 148     -10.924   4.952  44.801  1.00 42.59      A
ATOM   1138  N   ILE A 149      -8.897   5.270  45.715  1.00 41.44      A
ATOM   1139  CA  ILE A 149      -8.469   3.890  45.461  1.00 41.44      A
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FIGURE 25 CON'T

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ATOM   1140  CB  ILE A 149     -7.202   3.823  44.610  1.00 42.23      A
ATOM   1141  CG2 ILE A 149     -6.783   2.372  44.433  1.00 42.23      A
ATOM   1142  CG1 ILE A 149     -7.463   4.458  43.241  1.00 42.23      A
ATOM   1143  CD1 ILE A 149     -6.203   4.648  42.403  1.00 42.23      A
ATOM   1144  C   ILE A 149     -8.182   3.315  46.850  1.00 41.44      A
ATOM   1145  O   ILE A 149     -7.272   3.772  47.542  1.00 41.44      A
ATOM   1146  N   GLN A 150     -8.969   2.321  47.251  1.00 44.13      A
ATOM   1147  CA  GLN A 150     -8.842   1.730  48.578  1.00 44.13      A
ATOM   1148  CB  GLN A 150    -10.108   2.039  49.384  1.00 49.13      A
ATOM   1149  CG  GLN A 150    -10.094   1.579  50.835  1.00 49.13      A
ATOM   1150  CD  GLN A 150    -11.403   1.878  51.546  1.00 49.13      A
ATOM   1151  OE1 GLN A 150    -11.869   3.021  51.567  1.00 49.13      A
ATOM   1152  NE2 GLN A 150    -12.005   0.851  52.134  1.00 49.13      A
ATOM   1153  C   GLN A 150     -8.593   0.230  48.603  1.00 44.13      A
ATOM   1154  O   GLN A 150     -9.333  -0.551  47.997  1.00 44.13      A
ATOM   1155  N   SER A 151     -7.555  -0.174  49.325  1.00 46.94      A
ATOM   1156  CA  SER A 151     -7.243  -1.590  49.441  1.00 46.94      A
ATOM   1157  CB  SER A 151     -5.909  -1.799  50.168  1.00 41.30      A
ATOM   1158  OG  SER A 151     -5.680  -3.188  50.382  1.00 41.30      A
ATOM   1159  C   SER A 151     -8.352  -2.297  50.218  1.00 46.94      A
ATOM   1160  O   SER A 151     -8.877  -1.763  51.196  1.00 46.94      A
ATOM   1161  N   MSE A 152     -8.714  -3.491  49.769  1.00 54.87      A
ATOM   1162  CA  MSE A 152     -9.736  -4.279  50.443  1.00 54.87      A
ATOM   1163  CB  MSE A 152    -10.521  -5.115  49.422  1.00 70.62      A
ATOM   1164  CG  MSE A 152    -11.422  -4.294  48.492  1.00 70.62      A
ATOM   1165  SE  MSE A 152    -12.737  -3.231  49.456  1.00 70.62      A
ATOM   1166  CE  MSE A 152    -11.729  -1.594  49.615  1.00 70.62      A
ATOM   1167  C   MSE A 152     -9.043  -5.185  51.474  1.00 54.87      A
ATOM   1168  O   MSE A 152     -9.695  -5.909  52.229  1.00 54.87      A
ATOM   1169  N   LYS A 153     -7.712  -5.127  51.492  1.00 50.97      A
ATOM   1170  CA  LYS A 153     -6.897  -5.899  52.431  1.00 50.97      A
ATOM   1171  CB  LYS A 153     -5.841  -6.727  51.693  1.00 90.19      A
ATOM   1172  CG  LYS A 153     -6.356  -7.962  50.985  1.00 90.19      A
ATOM   1173  CD  LYS A 153     -5.197  -8.695  50.325  1.00 90.19      A
ATOM   1174  CE  LYS A 153     -5.638  -9.999  49.685  1.00 90.19      A
ATOM   1175  NZ  LYS A 153     -4.519 -10.624  48.923  1.00 90.19      A
ATOM   1176  C   LYS A 153     -6.179  -4.946  53.382  1.00 50.97      A
ATOM   1177  O   LYS A 153     -5.703  -3.885  52.973  1.00 50.97      A
ATOM   1178  N   THR A 154     -6.101  -5.326  54.651  1.00 48.31      A
ATOM   1179  CA  THR A 154     -5.426  -4.501  55.640  1.00 48.31      A

ATOM   1180  CB  THR A 154     -5.487  -5.139  57.047  1.00 46.93      A
ATOM   1181  OG1 THR A 154     -4.889  -6.442  56.996  1.00 46.93      A
ATOM   1182  CG2 THR A 154     -6.932  -5.248  57.539  1.00 46.93      A
ATOM   1183  C   THR A 154     -3.959  -4.381  55.247  1.00 48.31      A
ATOM   1184  O   THR A 154     -3.433  -5.224  54.524  1.00 48.31      A
ATOM   1185  N   LEU A 155     -3.306  -3.327  55.722  1.00 49.03      A
ATOM   1186  CA  LEU A 155     -1.896  -3.112  55.444  1.00 49.03      A
ATOM   1187  CB  LEU A 155     -1.424  -1.837  56.155  1.00 41.52      A
ATOM   1188  CG  LEU A 155      0.077  -1.527  56.127  1.00 41.52      A
ATOM   1189  CD1 LEU A 155      0.559  -1.395  54.671  1.00 41.52      A
ATOM   1190  CD2 LEU A 155      0.358  -0.244  56.912  1.00 41.52      A
ATOM   1191  C   LEU A 155     -1.082  -4.327  55.926  1.00 49.03      A
ATOM   1192  O   LEU A 155     -0.156  -4.778  55.249  1.00 49.03      A
ATOM   1193  N   TRP A 156     -1.440  -4.862  57.092  1.00 44.28      A
ATOM   1194  CA  TRP A 156     -0.730  -6.021  57.648  1.00 44.28      A
ATOM   1195  CB  TRP A 156     -1.290  -6.371  59.035  1.00 57.24      A
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FIGURE 25 CON'T

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ATOM   1196  CG  TRP A 156     -0.456  -7.355  59.831  1.00 57.24      A
ATOM   1197  CD2 TRP A 156      0.957  -7.288  60.091  1.00 57.24      A
ATOM   1198  CE2 TRP A 156      1.281  -8.380  60.931  1.00 57.24      A
ATOM   1199  CE3 TRP A 156      1.977  -6.413  59.700  1.00 57.24      A
ATOM   1200  CD1 TRP A 156     -0.912  -8.458  60.502  1.00 57.24      A
ATOM   1201  NE1 TRP A 156      0.124  -9.075  61.164  1.00 57.24      A
ATOM   1202  CZ2 TRP A 156      2.584  -8.619  61.388  1.00 57.24      A
ATOM   1203  CZ3 TRP A 156      3.277  -6.651  60.156  1.00 57.24      A
ATOM   1204  CH2 TRP A 156      3.566  -7.747  60.992  1.00 57.24      A
ATOM   1205  C   TRP A 156     -0.852  -7.227  56.709  1.00 44.28      A
ATOM   1206  O   TRP A 156      0.144  -7.898  56.424  1.00 44.28      A
ATOM   1207  N   GLU A 157     -2.066  -7.498  56.229  1.00 54.86      A
ATOM   1208  CA  GLU A 157     -2.292  -8.615  55.304  1.00 54.86      A
ATOM   1209  CB  GLU A 157     -3.791  -8.805  55.032  1.00 89.57      A
ATOM   1210  CG  GLU A 157     -4.613  -9.378  56.192  1.00 89.57      A
ATOM   1211  CD  GLU A 157     -4.183 -10.784  56.607  1.00 89.57      A
ATOM   1212  OE1 GLU A 157     -3.999 -11.649  55.722  1.00 89.57      A
ATOM   1213  OE2 GLU A 157     -4.041 -11.028  57.826  1.00 89.57      A
ATOM   1214  C   GLU A 157     -1.563  -8.404  53.968  1.00 54.86      A
ATOM   1215  O   GLU A 157     -1.016  -9.353  53.396  1.00 54.86      A
ATOM   1216  N   LEU A 158     -1.559  -7.166  53.474  1.00 65.79      A
ATOM   1217  CA  LEU A 158     -0.902  -6.843  52.203  1.00 65.79      A
ATOM   1218  CB  LEU A 158     -1.041  -5.350  51.858  1.00 58.91      A
ATOM   1219  CG  LEU A 158     -2.381  -4.781  51.380  1.00 58.91      A
ATOM   1220  CD1 LEU A 158     -2.184  -3.311  51.006  1.00 58.91      A
ATOM   1221  CD2 LEU A 158     -2.892  -5.567  50.166  1.00 58.91      A
ATOM   1222  C   LEU A 158      0.576  -7.183  52.202  1.00 65.79      A
ATOM   1223  O   LEU A 158      1.114  -7.635  51.194  1.00 65.79      A
ATOM   1224  N   VAL A 159      1.243  -6.951  53.326  1.00 53.76      A
ATOM   1225  CA  VAL A 159      2.667  -7.229  53.397  1.00 53.76      A
ATOM   1226  CB  VAL A 159      3.390  -6.165  54.245  1.00 42.90      A
ATOM   1227  CG1 VAL A 159      3.275  -4.826  53.567  1.00 42.90      A
ATOM   1228  CG2 VAL A 159      2.788  -6.089  55.654  1.00 42.90      A
ATOM   1229  C   VAL A 159      2.982  -8.621  53.927  1.00 53.76      A
ATOM   1230  O   VAL A 159      4.126  -8.924  54.260  1.00 53.76      A
ATOM   1231  N   ASN A 160      1.968  -9.474  53.989  1.00 60.19      A
ATOM   1232  CA  ASN A 160      2.155 -10.833  54.472  1.00 60.19      A
ATOM   1233  CB  ASN A 160      3.110 -11.585  53.546  1.00 75.15      A
ATOM   1234  CG  ASN A 160      2.628 -11.600  52.110  1.00 75.15      A
ATOM   1235  OD1 ASN A 160      1.543 -12.104  51.814  1.00 75.15      A
ATOM   1236  ND2 ASN A 160      3.432 -11.041  51.209  1.00 75.15      A
ATOM   1237  C   ASN A 160      2.686 -10.877  55.904  1.00 60.19      A
ATOM   1238  O   ASN A 160      3.582 -11.666  56.220  1.00 60.19      A
ATOM   1239  N   LYS A 161      2.133 -10.021  56.759  1.00 76.52      A
ATOM   1240  CA  LYS A 161      2.514  -9.969  58.168  1.00 76.52      A
ATOM   1241  CB  LYS A 161      1.879 -11.145  58.918  1.00 68.87      A
ATOM   1242  CG  LYS A 161      0.359 -11.203  58.856  1.00 68.87      A
ATOM   1243  CD  LYS A 161     -0.122 -12.637  59.038  1.00 68.87      A
ATOM   1244  CE  LYS A 161     -1.642 -12.751  59.103  1.00 68.87      A
ATOM   1245  NZ  LYS A 161     -2.174 -12.601  60.493  1.00 68.87      A
ATOM   1246  C   LYS A 161      4.025  -9.994  58.391  1.00 76.52      A
ATOM   1247  O   LYS A 161      4.496 -10.520  59.396  1.00 76.52      A
ATOM   1248  N   ASP A 162      4.786  -9.431  57.460  1.00 63.39      A
ATOM   1249  CA  ASP A 162      6.237  -9.412  57.602  1.00 63.39      A
ATOM   1250  CB  ASP A 162      6.905  -9.953  56.333  1.00 91.30      A
ATOM   1251  CG  ASP A 162      8.422  -9.923  56.413  1.00 91.30      A
ATOM   1252  OD1 ASP A 162      8.985 -10.438  57.402  1.00 91.30      A
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FIGURE 25 CON'T

ATOM	1253	OD2	ASP	A	162	9.053	-9.387	55.481	1.00	91.30	A
ATOM	1254	C	ASP	A	162	6.747	-8.006	57.897	1.00	63.39	A
ATOM	1255	O	ASP	A	162	6.662	-7.116	57.052	1.00	63.39	A
ATOM	1256	N	PRO	A	163	7.288	-7.789	59.109	1.00	61.09	A
ATOM	1257	CD	PRO	A	163	7.515	-8.786	60.172	1.00	64.53	A
ATOM	1258	CA	PRO	A	163	7.810	-6.477	59.506	1.00	61.09	A
ATOM	1259	CB	PRO	A	163	8.491	-6.766	60.843	1.00	64.53	A
ATOM	1260	CG	PRO	A	163	7.692	-7.911	61.391	1.00	64.53	A
ATOM	1261	C	PRO	A	163	8.794	-5.944	58.474	1.00	61.09	A
ATOM	1262	O	PRO	A	163	8.822	-4.743	58.191	1.00	61.09	A
ATOM	1263	N	LYS	A	164	9.593	-6.855	57.923	1.00	135.00	A
ATOM	1264	CA	LYS	A	164	10.599	-6.522	56.920	1.00	135.00	A
ATOM	1265	CB	LYS	A	164	11.804	-7.460	57.059	1.00	129.94	A
ATOM	1266	CG	LYS	A	164	13.137	-6.851	56.634	1.00	129.94	A
ATOM	1267	CD	LYS	A	164	13.131	-6.404	55.182	1.00	129.94	A
ATOM	1268	CE	LYS	A	164	14.456	-5.774	54.796	1.00	129.94	A
ATOM	1269	NZ	LYS	A	164	15.582	-6.728	54.973	1.00	129.94	A
ATOM	1270	C	LYS	A	164	10.004	-5.635	55.515	1.00	135.00	A
ATOM	1271	O	LYS	A	164	10.511	-7.359	54.658	1.00	135.00	A
ATOM	1272	N	GLU	A	165	8.913	-5.909	55.305	1.00	64.61	A
ATOM	1273	CA	GLU	A	165	8.196	-5.857	54.037	1.00	64.61	A
ATOM	1274	CB	GLU	A	165	7.451	-7.168	53.770	1.00	86.95	A
ATOM	1275	CG	GLU	A	165	6.534	-7.111	52.556	1.00	86.95	A
ATOM	1276	CD	GLU	A	165	6.123	-8.486	52.044	1.00	86.95	A
ATOM	1277	OE1	GLU	A	165	5.166	-8.559	51.242	1.00	86.95	A
ATOM	1278	OE2	GLU	A	165	6.760	-9.489	52.433	1.00	86.95	A
ATOM	1279	C	GLU	A	165	7.211	-4.709	54.210	1.00	64.61	A
ATOM	1280	O	GLU	A	165	6.870	-4.003	53.264	1.00	64.61	A
ATOM	1281	N	LEU	A	166	6.774	-4.536	55.452	1.00	51.26	A
ATOM	1282	CA	LEU	A	166	5.852	-3.478	55.829	1.00	51.26	A
ATOM	1283	CB	LEU	A	166	5.386	-3.704	57.273	1.00	79.12	A
ATOM	1284	CG	LEU	A	166	4.373	-2.777	57.951	1.00	79.12	A
ATOM	1285	CD1	LEU	A	166	4.037	-3.349	59.319	1.00	79.12	A
ATOM	1286	CD2	LEU	A	166	4.931	-1.378	58.104	1.00	79.12	A
ATOM	1287	C	LEU	A	166	6.599	-2.152	55.719	1.00	51.26	A
ATOM	1288	O	LEU	A	166	6.126	-1.203	55.091	1.00	51.26	A
ATOM	1289	N	GLU	A	167	7.773	-2.088	56.334	1.00	58.64	A
ATOM	1290	CA	GLU	A	167	8.564	-0.867	56.298	1.00	58.64	A
ATOM	1291	CB	GLU	A	167	9.827	-1.021	57.151	1.00	82.34	A
ATOM	1292	CG	GLU	A	167	10.730	0.203	57.131	1.00	82.34	A
ATOM	1293	CD	GLU	A	167	11.960	0.042	58.003	1.00	82.34	A
ATOM	1294	OE1	GLU	A	167	12.662	-0.982	57.856	1.00	82.34	A
ATOM	1295	OE2	GLU	A	167	12.227	0.943	58.829	1.00	82.34	A
ATOM	1296	C	GLU	A	167	8.944	-0.520	54.859	1.00	58.64	A
ATOM	1297	O	GLU	A	167	9.042	0.654	54.501	1.00	58.64	A
ATOM	1298	N	GLU	A	168	9.161	-1.545	54.039	1.00	64.16	A
ATOM	1299	CA	GLU	A	168	9.520	-1.331	52.643	1.00	64.16	A
ATOM	1300	CB	GLU	A	168	9.900	-2.657	51.971	1.00	106.41	A
ATOM	1301	CG	GLU	A	168	11.256	-3.215	52.395	1.00	106.41	A
ATOM	1302	CD	GLU	A	168	11.577	-4.551	51.739	1.00	106.41	A
ATOM	1303	OE1	GLU	A	168	11.561	-4.626	50.493	1.00	106.41	A
ATOM	1304	OE2	GLU	A	168	11.851	-5.528	52.470	1.00	106.41	A
ATOM	1305	C	GLU	A	168	8.335	-0.702	51.923	1.00	64.16	A
ATOM	1306	O	GLU	A	168	8.500	0.212	51.118	1.00	64.16	A
ATOM	1307	N	PHE	A	169	7.139	-1.195	52.232	1.00	55.37	A
ATOM	1308	CA	PHE	A	169	5.915	-0.684	51.628	1.00	55.37	A

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ATOM	1309	CB	PHE	A	169	4.706	-1.451	52.177	1.00	53.88	A
ATOM	1310	CG	PHE	A	169	3.415	-1.143	51.466	1.00	53.88	A
ATOM	1311	CD1	PHE	A	169	3.052	-1.845	50.316	1.00	53.88	A
ATOM	1312	CD2	PHE	A	169	2.567	-0.143	51.938	1.00	53.88	A
ATOM	1313	CE1	PHE	A	169	1.862	-1.556	49.649	1.00	53.88	A
ATOM	1314	CE2	PHE	A	169	1.374	0.157	51.279	1.00	53.88	A
ATOM	1315	CZ	PHE	A	169	1.018	-0.549	50.133	1.00	53.88	A
ATOM	1316	C	PHE	A	169	5.775	0.813	51.950	1.00	55.37	A
ATOM	1317	O	PHE	A	169	5.673	1.652	51.050	1.00	55.37	A
ATOM	1318	N	LEU	A	170	5.787	1.136	53.239	1.00	50.99	A
ATOM	1319	CA	LEU	A	170	5.656	2.518	53.696	1.00	50.99	A
ATOM	1320	CB	LEU	A	170	5.898	2.598	55.209	1.00	58.50	A
ATOM	1321	CG	LEU	A	170	4.683	2.588	56.149	1.00	58.50	A
ATOM	1322	CD1	LEU	A	170	3.532	1.796	55.560	1.00	58.50	A
ATOM	1323	CD2	LEU	A	170	5.112	2.012	57.490	1.00	58.50	A
ATOM	1324	C	LEU	A	170	6.602	3.466	52.982	1.00	50.99	A
ATOM	1325	O	LEU	A	170	6.200	4.541	52.553	1.00	50.99	A
ATOM	1326	N	MSE	A	171	7.858	3.052	52.859	1.00	63.39	A
ATOM	1327	CA	MSE	A	171	8.885	3.858	52.210	1.00	63.39	A
ATOM	1328	CB	MSE	A	171	10.254	3.196	52.393	1.00	80.35	A
ATOM	1329	CG	MSE	A	171	10.648	2.987	53.846	1.00	80.35	A
ATOM	1330	SE	MSE	A	171	12.434	2.258	54.064	1.00	80.35	A
ATOM	1331	CE	MSE	A	171	12.087	0.420	53.595	1.00	80.35	A
ATOM	1332	C	MSE	A	171	8.647	4.110	50.718	1.00	63.39	A
ATOM	1333	O	MSE	A	171	8.844	5.224	50.232	1.00	63.39	A
ATOM	1334	N	THR	A	172	8.232	3.073	49.998	1.00	62.45	A
ATOM	1335	CA	THR	A	172	8.001	3.187	48.564	1.00	62.45	A
ATOM	1336	CB	THR	A	172	7.875	1.800	47.902	1.00	87.89	A
ATOM	1337	OG1	THR	A	172	6.680	1.159	48.360	1.00	87.89	A
ATOM	1338	CG2	THR	A	172	9.075	0.931	48.247	1.00	87.89	A
ATOM	1339	C	THR	A	172	6.761	3.998	48.195	1.00	62.45	A
ATOM	1340	O	THR	A	172	6.779	4.736	47.213	1.00	62.45	A
ATOM	1341	N	HIS	A	173	5.692	3.865	48.980	1.00	52.70	A
ATOM	1342	CA	HIS	A	173	4.441	4.579	48.704	1.00	52.70	A
ATOM	1343	CB	HIS	A	173	3.254	3.647	48.936	1.00	59.03	A
ATOM	1344	CG	HIS	A	173	3.262	2.436	48.058	1.00	59.03	A
ATOM	1345	CD2	HIS	A	173	3.381	1.120	48.354	1.00	59.03	A
ATOM	1346	ND1	HIS	A	173	3.154	2.511	46.686	1.00	59.03	A
ATOM	1347	CE1	HIS	A	173	3.204	1.294	46.176	1.00	59.03	A
ATOM	1348	NE2	HIS	A	173	3.342	0.432	47.166	1.00	59.03	A
ATOM	1349	C	HIS	A	173	4.292	5.829	49.556	1.00	52.70	A
ATOM	1350	O	HIS	A	173	3.222	6.441	49.614	1.00	52.70	A
ATOM	1351	N	LYS	A	174	5.391	6.207	50.195	1.00	50.21	A
ATOM	1352	CA	LYS	A	174	5.441	7.361	51.087	1.00	50.21	A
ATOM	1353	CB	LYS	A	174	6.905	7.677	51.434	1.00	67.16	A
ATOM	1354	CG	LYS	A	174	7.128	9.042	52.091	1.00	67.16	A
ATOM	1355	CD	LYS	A	174	8.586	9.223	52.519	1.00	67.16	A
ATOM	1356	CE	LYS	A	174	8.982	10.701	52.637	1.00	67.16	A
ATOM	1357	NZ	LYS	A	174	8.142	11.497	53.570	1.00	67.16	A
ATOM	1358	C	LYS	A	174	4.755	8.639	50.615	1.00	50.21	A
ATOM	1359	O	LYS	A	174	3.994	9.249	51.366	1.00	50.21	A
ATOM	1360	N	GLU	A	175	5.034	9.040	49.379	1.00	50.65	A
ATOM	1361	CA	GLU	A	175	4.494	10.277	48.817	1.00	50.65	A
ATOM	1362	CB	GLU	A	175	5.123	10.533	47.444	1.00	95.83	A
ATOM	1363	CG	GLU	A	175	6.647	10.566	47.443	1.00	95.83	A
ATOM	1364	CD	GLU	A	175	7.220	11.504	48.494	1.00	95.83	A
ATOM	1365	OE1	GLU	A	175	6.744	12.656	48.594	1.00	95.83	A

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ATOM	1366	OE2	GLU	A	175	8.153	11.089	49.215	1.00	95.83	A
ATOM	1367	C	GLU	A	175	2.974	10.395	48.695	1.00	50.65	A
ATOM	1368	O	GLU	A	175	2.424	11.487	48.840	1.00	50.65	A
ATOM	1369	N	ASN	A	176	2.289	9.288	48.443	1.00	41.11	A
ATOM	1370	CA	ASN	A	176	0.839	9.349	48.283	1.00	41.11	A
ATOM	1371	CB	ASN	A	176	0.492	8.969	46.849	1.00	58.07	A
ATOM	1372	CG	ASN	A	176	1.348	9.699	45.841	1.00	58.07	A
ATOM	1373	OD1	ASN	A	176	1.352	10.927	45.792	1.00	58.07	A
ATOM	1374	ND2	ASN	A	176	2.085	8.949	45.035	1.00	58.07	A
ATOM	1375	C	ASN	A	176	0.010	8.481	49.239	1.00	41.11	A
ATOM	1376	O	ASN	A	176	-1.206	8.637	49.329	1.00	41.11	A
ATOM	1377	N	LEU	A	177	0.667	7.584	49.962	1.00	43.75	A
ATOM	1378	CA	LEU	A	177	-0.051	6.680	50.849	1.00	43.75	A
ATOM	1379	CB	LEU	A	177	0.891	5.602	51.381	1.00	45.30	A
ATOM	1380	CG	LEU	A	177	0.243	4.561	52.296	1.00	45.30	A
ATOM	1381	CD1	LEU	A	177	-0.659	3.666	51.469	1.00	45.30	A
ATOM	1382	CD2	LEU	A	177	1.322	3.732	52.998	1.00	45.30	A
ATOM	1383	C	LEU	A	177	-0.770	7.308	52.026	1.00	43.75	A
ATOM	1384	O	LEU	A	177	-0.230	8.153	52.744	1.00	43.75	A
ATOM	1385	N	MSE	A	178	-2.015	6.887	52.197	1.00	41.72	A
ATOM	1386	CA	MSE	A	178	-2.826	7.321	53.320	1.00	41.72	A
ATOM	1387	CB	MSE	A	178	-3.960	8.251	52.887	1.00	57.42	A
ATOM	1388	CG	MSE	A	178	-3.480	9.643	52.493	1.00	57.42	A
ATOM	1389	SE	MSE	A	178	-4.933	10.844	52.058	1.00	57.42	A
ATOM	1390	CE	MSE	A	178	-5.535	9.981	50.427	1.00	57.42	A
ATOM	1391	C	MSE	A	178	-3.366	6.017	53.886	1.00	41.72	A
ATOM	1392	O	MSE	A	178	-3.425	5.009	53.183	1.00	41.72	A
ATOM	1393	N	LEU	A	179	-3.732	6.034	55.160	1.00	41.26	A
ATOM	1394	CA	LEU	A	179	-4.234	4.841	55.817	1.00	41.26	A
ATOM	1395	CB	LEU	A	179	-3.202	4.351	56.835	1.00	39.11	A
ATOM	1396	CG	LEU	A	179	-1.915	3.859	56.180	1.00	39.11	A
ATOM	1397	CD1	LEU	A	179	-0.833	3.578	57.237	1.00	39.11	A
ATOM	1398	CD2	LEU	A	179	-2.244	2.605	55.371	1.00	39.11	A
ATOM	1399	C	LEU	A	179	-5.556	5.123	56.490	1.00	41.26	A
ATOM	1400	O	LEU	A	179	-5.667	6.054	57.282	1.00	41.26	A
ATOM	1401	N	LYS	A	180	-6.550	4.310	56.155	1.00	43.84	A
ATOM	1402	CA	LYS	A	180	-7.895	4.435	56.691	1.00	43.84	A
ATOM	1403	CB	LYS	A	180	-8.919	4.242	55.568	1.00	54.71	A
ATOM	1404	CG	LYS	A	180	-10.357	4.230	56.045	1.00	54.71	A
ATOM	1405	CD	LYS	A	180	-11.334	3.877	54.927	1.00	54.71	A
ATOM	1406	CE	LYS	A	180	-11.773	5.110	54.150	1.00	54.71	A
ATOM	1407	NZ	LYS	A	180	-10.607	5.837	53.579	1.00	54.71	A
ATOM	1408	C	LYS	A	180	-8.126	3.394	57.793	1.00	43.84	A
ATOM	1409	O	LYS	A	180	-7.940	2.197	57.581	1.00	43.84	A
ATOM	1410	N	ASP	A	181	-8.527	3.860	58.969	1.00	49.38	A
ATOM	1411	CA	ASP	A	181	-8.777	2.973	60.098	1.00	49.38	A
ATOM	1412	CB	ASP	A	181	-8.667	3.764	61.410	1.00	54.56	A
ATOM	1413	CG	ASP	A	181	-8.805	2.884	62.648	1.00	54.56	A
ATOM	1414	OD1	ASP	A	181	-8.441	3.347	63.753	1.00	54.56	A
ATOM	1415	OD2	ASP	A	181	-9.281	1.738	62.522	1.00	54.56	A
ATOM	1416	C	ASP	A	181	-10.167	2.356	59.956	1.00	49.38	A
ATOM	1417	O	ASP	A	181	-11.151	2.898	60.458	1.00	49.38	A
ATOM	1418	N	ILE	A	182	-10.243	1.224	59.264	1.00	52.94	A
ATOM	1419	CA	ILE	A	182	-11.520	0.553	59.066	1.00	52.94	A
ATOM	1420	CB	ILE	A	182	-11.441	-0.521	57.951	1.00	46.44	A
ATOM	1421	CG2	ILE	A	182	-11.239	0.144	56.593	1.00	46.44	A
ATOM	1422	CG1	ILE	A	182	-10.293	-1.489	58.228	1.00	46.44	A

ATOM	1423	CD1	ILE	A	182	-10.327	-2.717	57.343	1.00 46.44	A
ATOM	1424	C	ILE	A	182	-12.013	-0.111	60.353	1.00 52.94	A
ATOM	1425	O	ILE	A	182	-13.139	-0.600	60.417	1.00 52.94	A
ATOM	1426	N	ALA	A	183	-11.167	-0.135	61.376	1.00 63.47	A
ATOM	1427	CA	ALA	A	183	-11.559	-0.731	62.645	1.00 63.47	A
ATOM	1428	CB	ALA	A	183	-10.338	-1.238	63.385	1.00 49.82	A
ATOM	1429	C	ALA	A	183	-12.274	0.332	63.468	1.00 63.47	A
ATOM	1430	O	ALA	A	183	-12.640	0.102	64.620	1.00 63.47	A
ATOM	1431	N	SER	A	184	-12.466	1.501	62.863	1.00 73.28	A
ATOM	1432	CA	SER	A	184	-13.137	2.620	63.518	1.00 73.28	A
ATOM	1433	CB	SER	A	184	-12.217	3.844	63.538	1.00 66.59	A
ATOM	1434	OG	SER	A	184	-12.923	5.004	63.934	1.00 66.59	A
ATOM	1435	C	SER	A	184	-14.434	2.970	62.793	1.00 73.28	A
ATOM	1436	O	SER	A	184	-14.502	2.909	61.568	1.00 73.28	A
ATOM	1437	N	PRO	A	185	-15.481	3.342	63.546	1.00 71.36	A
ATOM	1438	CD	PRO	A	185	-15.533	3.473	65.012	1.00 73.07	A
ATOM	1439	CA	PRO	A	185	-16.770	3.697	62.947	1.00 71.36	A
ATOM	1440	CB	PRO	A	185	-17.687	3.820	64.159	1.00 73.07	A
ATOM	1441	CG	PRO	A	185	-16.764	4.325	65.213	1.00 73.07	A
ATOM	1442	C	PRO	A	185	-16.693	4.989	62.136	1.00 71.36	A
ATOM	1443	O	PRO	A	185	-17.577	5.277	61.329	1.00 71.36	A
ATOM	1444	N	LEU	A	186	-15.631	5.760	62.350	1.00 64.31	A
ATOM	1445	CA	LEU	A	186	-15.443	7.017	61.631	1.00 64.31	A
ATOM	1446	CB	LEU	A	186	-14.856	8.082	62.565	1.00 71.48	A
ATOM	1447	CG	LEU	A	186	-15.821	8.663	63.607	1.00 71.48	A
ATOM	1448	CD1	LEU	A	186	-15.070	9.585	64.555	1.00 71.48	A
ATOM	1449	CD2	LEU	A	186	-16.944	9.419	62.899	1.00 71.48	A
ATOM	1450	C	LEU	A	186	-14.555	6.867	60.395	1.00 64.31	A
ATOM	1451	O	LEU	A	186	-14.430	7.798	59.601	1.00 64.31	A
ATOM	1452	N	LYS	A	187	-13.948	5.695	60.232	1.00 57.82	A
ATOM	1453	CA	LYS	A	187	-13.078	5.437	59.087	1.00 57.82	A
ATOM	1454	CB	LYS	A	187	-13.910	5.246	57.816	1.00 72.64	A
ATOM	1455	CG	LYS	A	187	-14.565	3.884	57.699	1.00 72.64	A
ATOM	1456	CD	LYS	A	187	-15.571	3.645	58.800	1.00 72.64	A
ATOM	1457	CE	LYS	A	187	-16.206	2.267	58.671	1.00 72.64	A
ATOM	1458	NZ	LYS	A	187	-15.194	1.181	58.793	1.00 72.64	A
ATOM	1459	C	LYS	A	187	-12.102	6.586	58.883	1.00 57.82	A
ATOM	1460	O	LYS	A	187	-11.776	6.942	57.752	1.00 57.82	A
ATOM	1461	N	THR	A	188	-11.639	7.163	59.989	1.00 51.63	A
ATOM	1462	CA	THR	A	188	-10.706	8.278	59.934	1.00 51.63	A
ATOM	1463	CB	THR	A	188	-10.268	8.682	61.350	1.00 56.12	A
ATOM	1464	OG1	THR	A	188	-11.434	8.904	62.155	1.00 56.12	A
ATOM	1465	CG2	THR	A	188	-9.430	9.955	61.311	1.00 56.12	A
ATOM	1466	C	THR	A	188	-9.482	7.924	59.096	1.00 51.63	A
ATOM	1467	O	THR	A	188	-8.932	6.822	59.203	1.00 51.63	A
ATOM	1468	N	VAL	A	189	-9.064	8.870	58.261	1.00 52.14	A
ATOM	1469	CA	VAL	A	189	-7.920	8.687	57.373	1.00 52.14	A
ATOM	1470	CB	VAL	A	189	-8.211	9.301	55.989	1.00 43.84	A
ATOM	1471	CG1	VAL	A	189	-7.013	9.119	55.072	1.00 43.84	A
ATOM	1472	CG2	VAL	A	189	-9.458	8.654	55.395	1.00 43.84	A
ATOM	1473	C	VAL	A	189	-6.680	9.338	57.956	1.00 52.14	A
ATOM	1474	O	VAL	A	189	-6.745	10.449	58.468	1.00 52.14	A
ATOM	1475	N	TYR	A	190	-5.547	8.652	57.857	1.00 50.61	A
ATOM	1476	CA	TYR	A	190	-4.293	9.156	58.405	1.00 50.61	A
ATOM	1477	CB	TYR	A	190	-3.860	8.288	59.593	1.00 52.28	A
ATOM	1478	CG	TYR	A	190	-4.853	8.208	60.725	1.00 52.28	A

ATOM	1479	CD1	TYR	A	190	-4.700	8.995	61.872	1.00	52.28	A
ATOM	1480	CE1	TYR	A	190	-5.597	8.883	62.946	1.00	52.28	A
ATOM	1481	CD2	TYR	A	190	-5.928	7.316	60.672	1.00	52.28	A
ATOM	1482	CE2	TYR	A	190	-6.821	7.197	61.727	1.00	52.28	A
ATOM	1483	CZ	TYR	A	190	-6.649	7.980	62.862	1.00	52.28	A
ATOM	1484	OH	TYR	A	190	-7.519	7.842	63.916	1.00	52.28	A
ATOM	1485	C	TYR	A	190	-3.143	9.165	57.405	1.00	50.61	A
ATOM	1486	O	TYR	A	190	-3.209	8.524	56.352	1.00	50.61	A
ATOM	1487	N	LYS	A	191	-2.083	9.884	57.767	1.00	61.17	A
ATOM	1488	CA	LYS	A	191	-0.866	9.968	56.971	1.00	61.17	A
ATOM	1489	CB	LYS	A	191	-0.555	11.415	56.575	1.00	87.12	A
ATOM	1490	CG	LYS	A	191	-1.447	12.009	55.499	1.00	87.12	A
ATOM	1491	CD	LYS	A	191	-0.849	13.318	54.987	1.00	87.12	A
ATOM	1492	CE	LYS	A	191	-1.673	13.932	53.862	1.00	87.12	A
ATOM	1493	NZ	LYS	A	191	-2.996	14.428	54.329	1.00	87.12	A
ATOM	1494	C	LYS	A	191	0.253	9.456	57.874	1.00	61.17	A
ATOM	1495	O	LYS	A	191	0.530	10.040	58.918	1.00	61.17	A
ATOM	1496	N	PRO	A	192	0.911	8.359	57.488	1.00	58.43	A
ATOM	1497	CD	PRO	A	192	0.748	7.583	56.245	1.00	45.01	A
ATOM	1498	CA	PRO	A	192	1.996	7.826	58.324	1.00	58.43	A
ATOM	1499	CB	PRO	A	192	2.383	6.536	57.608	1.00	45.01	A
ATOM	1500	CG	PRO	A	192	2.068	6.855	56.155	1.00	45.01	A
ATOM	1501	C	PRO	A	192	3.178	8.789	58.475	1.00	58.43	A
ATOM	1502	O	PRO	A	192	3.603	9.409	57.501	1.00	58.43	A
ATOM	1503	N	CYS	A	193	3.695	8.908	59.702	1.00	55.22	A
ATOM	1504	CA	CYS	A	193	4.823	9.789	60.000	1.00	55.22	A
ATOM	1505	CB	CYS	A	193	4.886	10.104	61.494	1.00	68.19	A
ATOM	1506	SG	CYS	A	193	3.616	11.226	62.072	1.00	68.19	A
ATOM	1507	C	CYS	A	193	6.139	9.167	59.574	1.00	55.22	A
ATOM	1508	O	CYS	A	193	6.296	7.947	59.601	1.00	55.22	A
ATOM	1509	N	PHE	A	194	7.088	10.010	59.187	1.00	60.62	A
ATOM	1510	CA	PHE	A	194	8.387	9.531	58.740	1.00	60.62	A
ATOM	1511	CB	PHE	A	194	8.525	9.752	57.228	1.00	53.49	A
ATOM	1512	CG	PHE	A	194	7.899	8.667	56.400	1.00	53.49	A
ATOM	1513	CD1	PHE	A	194	8.615	7.514	56.089	1.00	53.49	A
ATOM	1514	CD2	PHE	A	194	6.586	8.784	55.953	1.00	53.49	A
ATOM	1515	CE1	PHE	A	194	8.029	6.486	55.340	1.00	53.49	A
ATOM	1516	CE2	PHE	A	194	5.990	7.767	55.204	1.00	53.49	A
ATOM	1517	CZ	PHE	A	194	6.711	6.617	54.897	1.00	53.49	A
ATOM	1518	C	PHE	A	194	9.550	10.203	59.461	1.00	60.62	A
ATOM	1519	O	PHE	A	194	9.435	11.340	59.932	1.00	60.62	A
ATOM	1520	N	GLU	A	195	10.664	9.480	59.548	1.00	69.72	A
ATOM	1521	CA	GLU	A	195	11.875	9.991	60.179	1.00	69.72	A
ATOM	1522	CB	GLU	A	195	13.003	8.965	60.048	1.00108.01		A
ATOM	1523	CG	GLU	A	195	13.893	8.837	61.269	1.00108.01		A
ATOM	1524	CD	GLU	A	195	13.215	8.091	62.401	1.00108.01		A
ATOM	1525	OE1	GLU	A	195	12.949	6.880	62.241	1.00108.01		A
ATOM	1526	OE2	GLU	A	195	12.944	8.715	63.449	1.00108.01		A
ATOM	1527	C	GLU	A	195	12.218	11.238	59.368	1.00	69.72	A
ATOM	1528	O	GLU	A	195	12.658	11.132	58.221	1.00	69.72	A
ATOM	1529	N	GLU	A	196	11.999	12.408	59.960	1.00	89.83	A
ATOM	1530	CA	GLU	A	196	12.249	13.685	59.293	1.00	89.83	A
ATOM	1531	CB	GLU	A	196	12.380	14.795	60.339	1.00117.08		A
ATOM	1532	CG	GLU	A	196	12.270	16.203	59.776	1.00117.08		A
ATOM	1533	CD	GLU	A	196	12.091	17.247	60.863	1.00117.08		A
ATOM	1534	OE1	GLU	A	196	12.999	17.395	61.708	1.00117.08		A
ATOM	1535	OE2	GLU	A	196	11.037	17.918	60.874	1,00117.08		A

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ATOM	1536	C	GLU	A	196	13.471	13.685	58.372	1.00	89.83	A
ATOM	1537	O	GLU	A	196	14.540	13.187	58.731	1.00	89.83	A
ATOM	1538	N	TYR	A	197	13.289	14.248	57.178	1.00	86.59	A
ATOM	1539	CA	TYR	A	197	14.341	14.339	56.167	1.00	86.59	A
ATOM	1540	CB	TYR	A	197	15.546	15.112	56.715	1.00	103.42	A
ATOM	1541	CG	TYR	A	197	15.226	16.507	57.201	1.00	103.42	A
ATOM	1542	CD1	TYR	A	197	14.431	17.365	56.444	1.00	103.42	A
ATOM	1543	CE1	TYR	A	197	14.167	18.665	56.868	1.00	103.42	A
ATOM	1544	CD2	TYR	A	197	15.750	16.984	58.402	1.00	103.42	A
ATOM	1545	CE2	TYR	A	197	15.494	18.284	58.834	1.00	103.42	A
ATOM	1546	CZ	TYR	A	197	14.702	19.118	58.062	1.00	103.42	A
ATOM	1547	OH	TYR	A	197	14.448	20.405	58.479	1.00	103.42	A
ATOM	1548	C	TYR	A	197	14.809	12.976	55.662	1.00	86.59	A
ATOM	1549	O	TYR	A	197	15.870	12.869	55.050	1.00	86.59	A
ATOM	1550	N	THR	A	198	14.011	11.940	55.910	1.00	70.57	A
ATOM	1551	CA	THR	A	198	14.356	10.585	55.487	1.00	70.57	A
ATOM	1552	CB	THR	A	198	15.005	9.800	56.664	1.00	81.15	A
ATOM	1553	OG1	THR	A	198	16.126	10.538	57.168	1.00	81.15	A
ATOM	1554	CG2	THR	A	198	15.490	8.433	56.212	1.00	81.15	A
ATOM	1555	C	THR	A	198	13.107	9.836	54.999	1.00	70.57	A
ATOM	1556	O	THR	A	198	12.001	10.383	55.000	1.00	70.57	A
ATOM	1557	N	LYS	A	199	13.292	8.590	54.569	1.00	70.64	A
ATOM	1558	CA	LYS	A	199	12.183	7.767	54.100	1.00	70.64	A
ATOM	1559	CB	LYS	A	199	12.505	7.150	52.734	1.00	111.90	A
ATOM	1560	CG	LYS	A	199	12.700	8.164	51.617	1.00	111.90	A
ATOM	1561	CD	LYS	A	199	12.939	7.479	50.277	1.00	111.90	A
ATOM	1562	CE	LYS	A	199	13.229	8.495	49.183	1.00	111.90	A
ATOM	1563	NZ	LYS	A	199	12.136	9.498	49.060	1.00	111.90	A
ATOM	1564	C	LYS	A	199	11.894	6.656	55.108	1.00	70.64	A
ATOM	1565	O	LYS	A	199	11.081	5.769	54.855	1.00	70.64	A
ATOM	1566	N	LYS	A	200	12.570	6.704	56.250	1.00	62.48	A
ATOM	1567	CA	LYS	A	200	12.361	5.698	57.287	1.00	62.48	A
ATOM	1568	CB	LYS	A	200	13.512	5.711	58.297	1.00	122.65	A
ATOM	1569	CG	LYS	A	200	13.367	4.668	59.399	1.00	122.65	A
ATOM	1570	CD	LYS	A	200	14.522	4.716	60.391	1.00	122.65	A
ATOM	1571	CE	LYS	A	200	15.844	4.330	59.739	1.00	122.65	A
ATOM	1572	NZ	LYS	A	200	16.978	4.341	60.711	1.00	122.65	A
ATOM	1573	C	LYS	A	200	11.048	5.994	57.998	1.00	62.48	A
ATOM	1574	O	LYS	A	200	10.874	7.062	58.580	1.00	62.48	A
ATOM	1575	N	PRO	A	201	10.094	5.055	57.944	1.00	53.04	A
ATOM	1576	CD	PRO	A	201	10.147	3.704	57.349	1.00	40.85	A
ATOM	1577	CA	PRO	A	201	8.810	5.288	58.613	1.00	53.04	A
ATOM	1578	CB	PRO	A	201	7.928	4.181	58.047	1.00	40.85	A
ATOM	1579	CG	PRO	A	201	8.896	3.034	57.929	1.00	40.85	A
ATOM	1580	C	PRO	A	201	8.977	5.173	60.134	1.00	53.04	A
ATOM	1581	O	PRO	A	201	9.802	4.387	60.614	1.00	53.04	A
ATOM	1582	N	LYS	A	202	8.210	5.955	60.886	1.00	62.83	A
ATOM	1583	CA	LYS	A	202	8.305	5.890	62.335	1.00	62.83	A
ATOM	1584	CB	LYS	A	202	7.868	7.220	62.958	1.00	80.05	A
ATOM	1585	CG	LYS	A	202	8.905	8.314	62.716	1.00	80.05	A
ATOM	1586	CD	LYS	A	202	8.771	9.507	63.650	1.00	80.05	A
ATOM	1587	CE	LYS	A	202	7.669	10.458	63.216	1.00	80.05	A
ATOM	1588	NZ	LYS	A	202	7.719	11.747	63.977	1.00	80.05	A
ATOM	1589	C	LYS	A	202	7.501	4.714	62.881	1.00	62.83	A
ATOM	1590	O	LYS	A	202	6.284	4.789	63.048	1.00	62.83	A
ATOM	1591	N	LEU	A	203	8.213	3.618	63.132	1.00	68.54	A

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ATOM	1592	CA	LEU	A	203	7.632	2.383	63.648	1.00	68.54	A
ATOM	1593	CB	LEU	A	203	8.010	1.216	62.729	1.00	68.04	A
ATOM	1594	CG	LEU	A	203	7.748	1.390	61.230	1.00	68.04	A
ATOM	1595	CD1	LEU	A	203	8.210	0.144	60.486	1.00	68.04	A
ATOM	1596	CD2	LEU	A	203	6.260	1.637	60.984	1.00	68.04	A
ATOM	1597	C	LEU	A	203	8.136	2.090	65.072	1.00	68.54	A
ATOM	1598	O	LEU	A	203	9.148	2.642	65.507	1.00	68.54	A
ATOM	1599	N	ASP	A	204	7.423	1.219	65.783	1.00	59.83	A
ATOM	1600	CA	ASP	A	204	7.779	0.829	67.149	1.00	59.83	A
ATOM	1601	CB	ASP	A	204	7.124	1.766	68.163	1.00	106.55	A
ATOM	1602	CG	ASP	A	204	7.654	3.175	68.073	1.00	106.55	A
ATOM	1603	OD1	ASP	A	204	8.859	3.374	68.335	1.00	106.55	A
ATOM	1604	OD2	ASP	A	204	6.869	4.084	67.735	1.00	106.55	A
ATOM	1605	C	ASP	A	204	7.292	-0.589	67.393	1.00	59.83	A
ATOM	1606	O	ASP	A	204	6.095	-0.860	67.296	1.00	59.83	A
ATOM	1607	N	HIS	A	205	8.216	-1.488	67.716	1.00	74.13	A
ATOM	1608	CA	HIS	A	205	7.864	-2.883	67.957	1.00	74.13	A
ATOM	1609	CB	HIS	A	205	9.041	-3.780	67.579	1.00	98.70	A
ATOM	1610	CG	HIS	A	205	9.165	-4.006	66.106	1.00	98.70	A
ATOM	1611	CD2	HIS	A	205	9.990	-3.455	65.184	1.00	98.70	A
ATOM	1612	ND1	HIS	A	205	8.335	-4.864	65.415	1.00	98.70	A
ATOM	1613	CE1	HIS	A	205	8.644	-4.830	64.131	1.00	98.70	A
ATOM	1614	NE2	HIS	A	205	9.644	-3.983	63.964	1.00	98.70	A
ATOM	1615	C	HIS	A	205	7.391	-3.209	69.371	1.00	74.13	A
ATOM	1616	O	HIS	A	205	7.172	-4.371	69.701	1.00	74.13	A
ATOM	1617	N	ASN	A	206	7.222	-2.181	70.194	1.00	61.62	A
ATOM	1618	CA	ASN	A	206	6.756	-2.352	71.568	1.00	61.62	A
ATOM	1619	CB	ASN	A	206	6.702	-0.991	72.269	1.00	64.76	A
ATOM	1620	CG	ASN	A	206	6.416	-1.105	73.756	1.00	64.76	A
ATOM	1621	OD1	ASN	A	206	5.841	-2.091	74.222	1.00	64.76	A
ATOM	1622	ND2	ASN	A	206	6.804	-0.081	74.508	1.00	64.76	A
ATOM	1623	C	ASN	A	206	5.361	-2.993	71.594	1.00	61.62	A
ATOM	1624	O	ASN	A	206	4.366	-2.356	71.239	1.00	61.62	A
ATOM	1625	N	GLN	A	207	5.299	-4.250	72.029	1.00	53.30	A
ATOM	1626	CA	GLN	A	207	4.041	-4.994	72.114	1.00	53.30	A
ATOM	1627	CB	GLN	A	207	4.310	-6.422	72.598	1.00	74.58	A
ATOM	1628	CG	GLN	A	207	5.065	-7.282	71.602	1.00	74.58	A
ATOM	1629	CD	GLN	A	207	5.256	-8.708	72.089	1.00	74.58	A
ATOM	1630	OE1	GLN	A	207	4.338	-9.314	72.645	1.00	74.58	A
ATOM	1631	NE2	GLN	A	207	6.446	-9.256	71.866	1.00	74.58	A
ATOM	1632	C	GLN	A	207	2.992	-4.345	73.018	1.00	53.30	A
ATOM	1633	O	GLN	A	207	1.801	-4.641	72.903	1.00	53.30	A
ATOM	1634	N	GLU	A	208	3.423	-3.469	73.923	1.00	52.45	A
ATOM	1635	CA	GLU	A	208	2.474	-2.806	74.810	1.00	52.45	A
ATOM	1636	CB	GLU	A	208	3.200	-2.119	75.969	1.00	63.72	A
ATOM	1637	CG	GLU	A	208	3.997	-3.068	76.853	1.00	63.72	A
ATOM	1638	CD	GLU	A	208	3.163	-4.218	77.383	1.00	63.72	A
ATOM	1639	OE1	GLU	A	208	2.130	-3.954	78.038	1.00	63.72	A
ATOM	1640	OE2	GLU	A	208	3.544	-5.386	77.144	1.00	63.72	A
ATOM	1641	C	GLU	A	208	1.677	-1.777	74.020	1.00	52.45	A
ATOM	1642	O	GLU	A	208	0.462	-1.648	74.190	1.00	52.45	A
ATOM	1643	N	ILE	A	209	2.366	-1.037	73.154	1.00	47.68	A
ATOM	1644	CA	ILE	A	209	1.694	-0.034	72.327	1.00	47.68	A
ATOM	1645	CB	ILE	A	209	2.665	0.669	71.360	1.00	60.91	A
ATOM	1646	CG2	ILE	A	209	1.912	1.732	70.575	1.00	60.91	A
ATOM	1647	CG1	ILE	A	209	3.821	1.307	72.133	1.00	60.91	A
ATOM	1648	CD1	ILE	A	209	4.913	1.897	71.236	1.00	60.91	A

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ATOM	1649	C	ILE	A	209	0.632	-0.740	71.488	1.00	47.68	A
ATOM	1650	O	ILE	A	209	-0.519	-0.314	71.437	1.00	47.68	A
ATOM	1651	N	VAL	A	210	1.034	-1.837	70.852	1.00	51.01	A
ATOM	1652	CA	VAL	A	210	0.130	-2.603	70.001	1.00	51.01	A
ATOM	1653	CB	VAL	A	210	0.850	-3.803	69.355	1.00	51.75	A
ATOM	1654	CG1	VAL	A	210	-0.140	-4.636	68.539	1.00	51.75	A
ATOM	1655	CG2	VAL	A	210	1.965	-3.305	68.464	1.00	51.75	A
ATOM	1656	C	VAL	A	210	-1.082	-3.109	70.766	1.00	51.01	A
ATOM	1657	O	VAL	A	210	-2.219	-2.886	70.355	1.00	51.01	A
ATOM	1658	N	LYS	A	211	-0.841	-3.786	71.882	1.00	51.09	A
ATOM	1659	CA	LYS	A	211	-1.935	-4.312	72.692	1.00	51.09	A
ATOM	1660	CB	LYS	A	211	-1.381	-5.026	73.930	1.00	107.12	A
ATOM	1661	CG	LYS	A	211	-2.448	-5.719	74.768	1.00	107.12	A
ATOM	1662	CD	LYS	A	211	-3.215	-6.751	73.945	1.00	107.12	A
ATOM	1663	CE	LYS	A	211	-4.386	-7.338	74.720	1.00	107.12	A
ATOM	1664	NZ	LYS	A	211	-5.135	-8.342	73.912	1.00	107.12	A
ATOM	1665	C	LYS	A	211	-2.894	-3.200	73.119	1.00	51.09	A
ATOM	1666	O	LYS	A	211	-4.116	-3.309	72.951	1.00	51.09	A
ATOM	1667	N	TYR	A	212	-2.332	-2.120	73.652	1.00	49.34	A
ATOM	1668	CA	TYR	A	212	-3.137	-0.999	74.116	1.00	49.34	A
ATOM	1669	CB	TYR	A	212	-2.250	0.135	74.633	1.00	56.43	A
ATOM	1670	CG	TYR	A	212	-3.056	1.308	75.153	1.00	56.43	A
ATOM	1671	CD1	TYR	A	212	-3.607	1.293	76.443	1.00	56.43	A
ATOM	1672	CE1	TYR	A	212	-4.403	2.349	76.906	1.00	56.43	A
ATOM	1673	CD2	TYR	A	212	-3.318	2.412	74.339	1.00	56.43	A
ATOM	1674	CE2	TYR	A	212	-4.110	3.470	74.790	1.00	56.43	A
ATOM	1675	CZ	TYR	A	212	-4.651	3.432	76.072	1.00	56.43	A
ATOM	1676	OH	TYR	A	212	-5.451	4.472	76.498	1.00	56.43	A
ATOM	1677	C	TYR	A	212	-4.078	-0.430	73.063	1.00	49.34	A
ATOM	1678	O	TYR	A	212	-5.290	-0.351	73.283	1.00	49.34	A
ATOM	1679	N	TRP	A	213	-3.530	-0.015	71.922	1.00	53.75	A
ATOM	1680	CA	TRP	A	213	-4.372	0.566	70.883	1.00	53.75	A
ATOM	1681	CB	TRP	A	213	-3.507	1.327	69.876	1.00	45.29	A
ATOM	1682	CG	TRP	A	213	-2.937	2.567	70.517	1.00	45.29	A
ATOM	1683	CD2	TRP	A	213	-3.680	3.696	71.002	1.00	45.29	A
ATOM	1684	CE2	TRP	A	213	-2.751	4.594	71.572	1.00	45.29	A
ATOM	1685	CE3	TRP	A	213	-5.042	4.034	71.011	1.00	45.29	A
ATOM	1686	CD1	TRP	A	213	-1.624	2.820	70.805	1.00	45.29	A
ATOM	1687	NE1	TRP	A	213	-1.506	4.035	71.440	1.00	45.29	A
ATOM	1688	CZ2	TRP	A	213	-3.138	5.811	72.146	1.00	45.29	A
ATOM	1689	CZ3	TRP	A	213	-5.429	5.248	71.582	1.00	45.29	A
ATOM	1690	CH2	TRP	A	213	-4.476	6.121	72.141	1.00	45.29	A
ATOM	1691	C	TRP	A	213	-5.309	-0.427	70.204	1.00	53.75	A
ATOM	1692	O	TRP	A	213	-6.370	-0.042	69.710	1.00	53.75	A
ATOM	1693	N	TYR	A	214	-4.938	-1.703	70.191	1.00	46.49	A
ATOM	1694	CA	TYR	A	214	-5.824	-2.713	69.614	1.00	46.49	A
ATOM	1695	CB	TYR	A	214	-5.120	-4.067	69.522	1.00	46.14	A
ATOM	1696	CG	TYR	A	214	-6.029	-5.212	69.116	1.00	46.14	A
ATOM	1697	CD1	TYR	A	214	-5.952	-5.772	67.843	1.00	46.14	A
ATOM	1698	CE1	TYR	A	214	-6.763	-6.850	67.478	1.00	46.14	A
ATOM	1699	CD2	TYR	A	214	-6.950	-5.756	70.020	1.00	46.14	A
ATOM	1700	CE2	TYR	A	214	-7.768	-6.830	69.666	1.00	46.14	A
ATOM	1701	CZ	TYR	A	214	-7.666	-7.376	68.393	1.00	46.14	A
ATOM	1702	OH	TYR	A	214	-8.447	-8.462	68.046	1.00	46.14	A
ATOM	1703	C	TYR	A	214	-7.023	-2.823	70.562	1.00	46.49	A
ATOM	1704	O	TYR	A	214	-8.180	-2.791	70.135	1.00	46.49	A

FIGURE 25 CON'T
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ATOM   1705  N   ASN A 215     -6.737  -2.954  71.857  1.00 53.54      A
ATOM   1706  CA  ASN A 215     -7.797  -3.057  72.854  1.00 53.54      A
ATOM   1707  CB  ASN A 215     -7.199  -3.338  74.237  1.00 73.57      A
ATOM   1708  CG  ASN A 215     -8.211  -3.167  75.357  1.00 73.57      A
ATOM   1709  OD1 ASN A 215     -8.447  -2.052  75.836  1.00 73.57      A
ATOM   1710  ND2 ASN A 215     -8.828  -4.272  75.770  1.00 73.57      A
ATOM   1711  C   ASN A 215     -8.627  -1.778  72.889  1.00 53.54      A
ATOM   1712  O   ASN A 215     -9.838  -1.813  73.117  1.00 53.54      A
ATOM   1713  N   TYR A 216     -7.970  -0.650  72.657  1.00 55.91      A
ATOM   1714  CA  TYR A 216     -8.656   0.635  72.650  1.00 55.91      A
ATOM   1715  CB  TYR A 216     -7.697   1.746  72.236  1.00 71.73      A
ATOM   1716  CG  TYR A 216     -8.340   3.111  72.213  1.00 71.73      A
ATOM   1717  CD1 TYR A 216     -8.384   3.901  73.363  1.00 71.73      A
ATOM   1718  CE1 TYR A 216     -8.981   5.161  73.349  1.00 71.73      A
ATOM   1719  CD2 TYR A 216     -8.915   3.612  71.045  1.00 71.73      A
ATOM   1720  CE2 TYR A 216     -9.519   4.870  71.018  1.00 71.73      A
ATOM   1721  CZ  TYR A 216     -9.547   5.640  72.174  1.00 71.73      A
ATOM   1722  OH  TYR A 216    -10.130   6.889  72.158  1.00 71.73      A
ATOM   1723  C   TYR A 216     -9.866   0.652  71.705  1.00 55.91      A
ATOM   1724  O   TYR A 216    -10.932   1.155  72.068  1.00 55.91      A
ATOM   1725  N   HIS A 217     -9.703   0.124  70.492  1.00 53.08      A
ATOM   1726  CA  HIS A 217    -10.810   0.116  69.533  1.00 53.08      A
ATOM   1727  CB  HIS A 217    -10.401  -0.505  68.187  1.00 46.99      A
ATOM   1728  CG  HIS A 217     -9.496   0.356  67.368  1.00 46.99      A
ATOM   1729  CD2 HIS A 217     -9.754   1.180  66.324  1.00 46.99      A
ATOM   1730  ND1 HIS A 217     -8.143   0.453  67.608  1.00 46.99      A
ATOM   1731  CE1 HIS A 217     -7.606   1.300  66.747  1.00 46.99      A
ATOM   1732  NE2 HIS A 217     -8.561   1.755  65.957  1.00 46.99      A
ATOM   1733  C   HIS A 217    -12.006  -0.653  70.064  1.00 53.08      A
ATOM   1734  O   HIS A 217    -13.141  -0.198  69.962  1.00 53.08      A
ATOM   1735  N   ILE A 218    -11.748  -1.827  70.620  1.00 54.18      A
ATOM   1736  CA  ILE A 218    -12.822  -2.650  71.145  1.00 54.18      A
ATOM   1737  CB  ILE A 218    -12.283  -4.022  71.561  1.00 55.73      A
ATOM   1738  CG2 ILE A 218    -13.388  -4.843  72.200  1.00 55.73      A
ATOM   1739  CG1 ILE A 218    -11.712  -4.726  70.322  1.00 55.73      A
ATOM   1740  CD1 ILE A 218    -11.023  -6.035  70.598  1.00 55.73      A
ATOM   1741  C   ILE A 218    -13.549  -1.978  72.310  1.00 54.18      A
ATOM   1742  O   ILE A 218    -14.770  -1.846  72.284  1.00 54.18      A
ATOM   1743  N   GLU A 219    -12.800  -1.533  73.314  1.00 75.71      A
ATOM   1744  CA  GLU A 219    -13.391  -0.870  74.477  1.00 75.71      A
ATOM   1745  CB  GLU A 219    -12.291  -0.406  75.440  1.00 74.86      A
ATOM   1746  CG  GLU A 219    -12.088  -1.299  76.651  1.00 74.86      A
ATOM   1747  CD  GLU A 219    -13.337  -1.411  77.510  1.00 74.86      A
ATOM   1748  OE1 GLU A 219    -13.868  -0.365  77.939  1.00 74.86      A
ATOM   1749  OE2 GLU A 219    -13.786  -2.551  77.755  1.00 74.86      A
ATOM   1750  C   GLU A 219    -14.259   0.338  74.125  1.00 75.71      A
ATOM   1751  O   GLU A 219    -15.378   0.481  74.620  1.00 75.71      A
ATOM   1752  N   ARG A 220    -13.730   1.206  73.271  1.00 74.22      A
ATOM   1753  CA  ARG A 220    -14.419   2.427  72.872  1.00 74.22      A
ATOM   1754  CB  ARG A 220    -13.365   3.489  72.525  1.00 98.22      A
ATOM   1755  CG  ARG A 220    -13.686   4.347  71.317  1.00 98.22      A
ATOM   1756  CD  ARG A 220    -14.576   5.526  71.649  1.00 98.22      A
ATOM   1757  NE  ARG A 220    -13.799   6.686  72.076  1.00 98.22      A
ATOM   1758  CZ  ARG A 220    -14.275   7.926  72.113  1.00 98.22      A
ATOM   1759  NH1 ARG A 220    -15.527   8.169  71.747  1.00 98.22      A
ATOM   1760  NH2 ARG A 220    -13.498   8.926  72.508  1.00 98.22      A
ATOM   1761  C   ARG A 220    -15.452   2.316  71.738  1.00 74.22      A
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ATOM	1762	O	ARG	A	220	-16.399	3.102	71.691	1.00	74.22	A
ATOM	1763	N	TYR	A	221	-15.299	1.349	70.840	1.00	70.93	A
ATOM	1764	CA	TYR	A	221	-16.241	1.249	69.725	1.00	70.93	A
ATOM	1765	CB	TYR	A	221	-15.500	1.446	68.401	1.00	67.88	A
ATOM	1766	CG	TYR	A	221	-14.785	2.770	68.281	1.00	67.88	A
ATOM	1767	CD1	TYR	A	221	-15.483	3.975	68.377	1.00	67.88	A
ATOM	1768	CE1	TYR	A	221	-14.828	5.200	68.244	1.00	67.88	A
ATOM	1769	CD2	TYR	A	221	-13.412	2.820	68.051	1.00	67.88	A
ATOM	1770	CE2	TYR	A	221	-12.748	4.033	67.919	1.00	67.88	A
ATOM	1771	CZ	TYR	A	221	-13.460	5.219	68.015	1.00	67.88	A
ATOM	1772	OH	TYR	A	221	-12.797	6.417	67.882	1.00	67.88	A
ATOM	1773	C	TYR	A	221	-17.115	0.008	69.601	1.00	70.93	A
ATOM	1774	O	TYR	A	221	-18.255	0.109	69.154	1.00	70.93	A
ATOM	1775	N	TRP	A	222	-16.599	-1.158	69.972	1.00	62.80	A
ATOM	1776	CA	TRP	A	222	-17.383	-2.384	69.846	1.00	62.80	A
ATOM	1777	CB	TRP	A	222	-16.775	-3.286	68.767	1.00	91.59	A
ATOM	1778	CG	TRP	A	222	-16.252	-2.534	67.584	1.00	91.59	A
ATOM	1779	CD2	TRP	A	222	-17.017	-2.014	66.490	1.00	91.59	A
ATOM	1780	CE2	TRP	A	222	-16.119	-1.333	65.640	1.00	91.59	A
ATOM	1781	CE3	TRP	A	222	-18.375	-2.056	66.146	1.00	91.59	A
ATOM	1782	CD1	TRP	A	222	-14.959	-2.160	67.359	1.00	91.59	A
ATOM	1783	NE1	TRP	A	222	-14.870	-1.438	66.194	1.00	91.59	A
ATOM	1784	CZ2	TRP	A	222	-16.534	-0.696	64.466	1.00	91.59	A
ATOM	1785	CZ3	TRP	A	222	-18.789	-1.423	64.979	1.00	91.59	A
ATOM	1786	CH2	TRP	A	222	-17.869	-0.752	64.153	1.00	91.59	A
ATOM	1787	C	TRP	A	222	-17.468	-3.154	71.153	1.00	62.80	A
ATOM	1788	O	TRP	A	222	-17.245	-4.366	71.178	1.00	62.80	A
ATOM	1789	N	ASN	A	223	-17.813	-2.452	72.228	1.00	84.04	A
ATOM	1790	CA	ASN	A	223	-17.910	-3.055	73.555	1.00	84.04	A
ATOM	1791	CB	ASN	A	223	-17.825	-1.958	74.623	1.00	128.47	A
ATOM	1792	CG	ASN	A	223	-17.529	-2.507	76.007	1.00	128.47	A
ATOM	1793	OD1	ASN	A	223	-18.229	-3.387	76.504	1.00	128.47	A
ATOM	1794	ND2	ASN	A	223	-16.486	-1.982	76.638	1.00	128.47	A
ATOM	1795	C	ASN	A	223	-19.182	-3.882	73.773	1.00	84.04	A
ATOM	1796	O	ASN	A	223	-19.931	-3.642	74.717	1.00	84.04	A
ATOM	1797	N	THR	A	224	-19.430	-4.849	72.898	1.00	66.05	A
ATOM	1798	CA	THR	A	224	-20.603	-5.707	73.029	1.00	66.05	A
ATOM	1799	CB	THR	A	224	-21.816	-5.168	72.235	1.00	84.17	A
ATOM	1800	OG1	THR	A	224	-21.571	-5.309	70.832	1.00	84.17	A
ATOM	1801	CG2	THR	A	224	-22.063	-3.702	72.555	1.00	84.17	A
ATOM	1802	C	THR	A	224	-20.251	-7.087	72.486	1.00	66.05	A
ATOM	1803	O	THR	A	224	-19.498	-7.211	71.520	1.00	66.05	A
ATOM	1804	N	PRO	A	225	-20.785	-8.148	73.105	1.00	84.76	A
ATOM	1805	CD	PRO	A	225	-21.668	-8.182	74.286	1.00	62.62	A
ATOM	1806	CA	PRO	A	225	-20.486	-9.502	72.635	1.00	84.76	A
ATOM	1807	CB	PRO	A	225	-21.483	-10.355	73.412	1.00	62.62	A
ATOM	1808	CG	PRO	A	225	-21.568	-9.626	74.723	1.00	62.62	A
ATOM	1809	C	PRO	A	225	-20.623	-9.668	71.116	1.00	84.76	A
ATOM	1810	O	PRO	A	225	-19.780	-10.292	70.469	1.00	84.76	A
ATOM	1811	N	GLU	A	226	-21.682	-9.099	70.550	1.00	72.64	A
ATOM	1812	CA	GLU	A	226	-21.916	-9.211	69.117	1.00	72.64	A
ATOM	1813	CB	GLU	A	226	-23.335	-8.747	68.782	1.00	147.05	A
ATOM	1814	CG	GLU	A	226	-24.414	-9.534	69.507	1.00	147.05	A
ATOM	1815	CD	GLU	A	226	-25.810	-9.198	69.023	1.00	147.05	A
ATOM	1816	OE1	GLU	A	226	-26.196	-8.012	69.085	1.00	147.05	A
ATOM	1817	OE2	GLU	A	226	-26.523	-10.125	68.583	1.00	147.05	A
ATOM	1818	C	GLU	A	226	-20.898	-8.420	68.303	1.00	72.64	A

FIGURE 25 CONT

ATOM	1819	O	GLU	A	226	-20.334	-8.931	67.333	1.00	72.64	A
ATOM	1820	N	ALA	A	227	-20.660	-7.173	68.694	1.00	77.94	A
ATOM	1821	CA	ALA	A	227	-19.699	-6.344	67.979	1.00	77.94	A
ATOM	1822	CB	ALA	A	227	-19.760	-4.910	68.490	1.00	58.35	A
ATOM	1823	C	ALA	A	227	-18.288	-6.914	68.142	1.00	77.94	A
ATOM	1824	O	ALA	A	227	-17.491	-6.896	67.203	1.00	77.94	A
ATOM	1825	N	LYS	A	228	-17.996	-7.430	69.335	1.00	58.30	A
ATOM	1826	CA	LYS	A	228	-16.694	-8.016	69.635	1.00	58.30	A
ATOM	1827	CB	LYS	A	228	-16.630	-8.483	71.090	1.00	76.00	A
ATOM	1828	CG	LYS	A	228	-16.501	-7.399	72.136	1.00	76.00	A
ATOM	1829	CD	LYS	A	228	-16.430	-8.034	73.520	1.00	76.00	A
ATOM	1830	CE	LYS	A	228	-16.311	-6.996	74.620	1.00	76.00	A
ATOM	1831	NZ	LYS	A	228	-16.287	-7.636	75.966	1.00	76.00	A
ATOM	1832	C	LYS	A	228	-16.431	-9.220	68.749	1.00	58.30	A
ATOM	1833	O	LYS	A	228	-15.311	-9.432	68.280	1.00	58.30	A
ATOM	1834	N	LEU	A	229	-17.469	-10.022	68.545	1.00	61.22	A
ATOM	1835	CA	LEU	A	229	-17.350	-11.218	67.731	1.00	61.22	A
ATOM	1836	CB	LEU	A	229	-18.655	-12.015	67.770	1.00	70.56	A
ATOM	1837	CG	LEU	A	229	-18.560	-13.534	67.604	1.00	70.56	A
ATOM	1838	CD1	LEU	A	229	-19.956	-14.073	67.339	1.00	70.56	A
ATOM	1839	CD2	LEU	A	229	-17.628	-13.907	66.466	1.00	70.56	A
ATOM	1840	C	LEU	A	229	-17.035	-10.829	66.292	1.00	61.22	A
ATOM	1841	O	LEU	A	229	-16.155	-11.413	65.663	1.00	61.22	A
ATOM	1842	N	GLU	A	230	-17.759	-9.841	65.774	1.00	65.81	A
ATOM	1843	CA	GLU	A	230	-17.542	-9.400	64.405	1.00	65.81	A
ATOM	1844	CB	GLU	A	230	-18.571	-8.339	64.012	1.00	111.18	A
ATOM	1845	CG	GLU	A	230	-18.604	-8.063	62.517	1.00	111.18	A
ATOM	1846	CD	GLU	A	230	-19.660	-7.048	62.128	1.00	111.18	A
ATOM	1847	OE1	GLU	A	230	-20.849	-7.269	62.446	1.00	111.18	A
ATOM	1848	OE2	GLU	A	230	-19.300	-6.030	61.500	1.00	111.18	A
ATOM	1849	C	GLU	A	230	-16.134	-8.839	64.263	1.00	65.81	A
ATOM	1850	O	GLU	A	230	-15.428	-9.133	63.293	1.00	65.81	A
ATOM	1851	N	PHE	A	231	-15.726	-8.039	65.243	1.00	56.50	A
ATOM	1852	CA	PHE	A	231	-14.399	-7.446	65.228	1.00	56.50	A
ATOM	1853	CB	PHE	A	231	-14.155	-6.654	66.509	1.00	59.08	A
ATOM	1854	CG	PHE	A	231	-12.802	-6.010	66.570	1.00	59.08	A
ATOM	1855	CD1	PHE	A	231	-12.615	-4.712	66.117	1.00	59.08	A
ATOM	1856	CD2	PHE	A	231	-11.707	-6.714	67.065	1.00	59.08	A
ATOM	1857	CE1	PHE	A	231	-11.355	-4.121	66.157	1.00	59.08	A
ATOM	1858	CE2	PHE	A	231	-10.447	-6.132	67.107	1.00	59.08	A
ATOM	1859	CZ	PHE	A	231	-10.270	-4.834	66.654	1.00	59.08	A
ATOM	1860	C	PHE	A	231	-13.350	-8.544	65.097	1.00	56.50	A
ATOM	1861	O	PHE	A	231	-12.457	-8.467	64.247	1.00	56.50	A
ATOM	1862	N	TYR	A	232	-13.456	-9.572	65.933	1.00	57.07	A
ATOM	1863	CA	TYR	A	232	-12.497	-10.677	65.879	1.00	57.07	A
ATOM	1864	CB	TYR	A	232	-12.660	-11.578	67.106	1.00	68.47	A
ATOM	1865	CG	TYR	A	232	-11.837	-11.108	68.282	1.00	68.47	A
ATOM	1866	CD1	TYR	A	232	-10.530	-11.550	68.458	1.00	68.47	A
ATOM	1867	CE1	TYR	A	232	-9.748	-11.085	69.507	1.00	68.47	A
ATOM	1868	CD2	TYR	A	232	-12.348	-10.183	69.192	1.00	68.47	A
ATOM	1869	CE2	TYR	A	232	-11.575	-9.709	70.246	1.00	68.47	A
ATOM	1870	CZ	TYR	A	232	-10.274	-10.165	70.398	1.00	68.47	A
ATOM	1871	OH	TYR	A	232	-9.497	-9.695	71.437	1.00	68.47	A
ATOM	1872	C	TYR	A	232	-12.620	-11.491	64.593	1.00	57.07	A
ATOM	1873	O	TYR	A	232	-11.637	-12.060	64.109	1.00	57.07	A
ATOM	1874	N	ARG	A	233	-13.823	-11.545	64.035	1.00	65.42	A

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ATOM   1875  CA  ARG A 233     -14.023 -12.274  62.787  1.00 65.42      A
ATOM   1876  CB  ARG A 233     -15.513 -12.396  62.452  1.00 90.05      A
ATOM   1877  CG  ARG A 233     -16.302 -13.367  63.310  1.00 90.05      A
ATOM   1878  CD  ARG A 233     -17.130 -14.284  62.422  1.00 90.05      A
ATOM   1879  NE  ARG A 233     -18.264 -14.885  63.118  1.00 90.05      A
ATOM   1880  CZ  ARG A 233     -19.316 -14.203  63.561  1.00 90.05      A
ATOM   1881  NH1 ARG A 233     -19.383 -12.888  63.385  1.00 90.05      A
ATOM   1882  NH2 ARG A 233     -20.308 -14.837  64.170  1.00 90.05      A
ATOM   1883  C   ARG A 233     -13.329 -11.515  61.658  1.00 65.42      A
ATOM   1884  O   ARG A 233     -12.673 -12.109  60.804  1.00 65.42      A
ATOM   1885  N   LYS A 234     -13.475 -10.194  61.677  1.00 66.11      A
ATOM   1886  CA  LYS A 234     -12.899  -9.327  60.654  1.00 66.11      A
ATOM   1887  CB  LYS A 234     -13.600  -7.964  60.689  1.00 82.51      A
ATOM   1888  CG  LYS A 234     -13.204  -7.020  59.569  1.00 82.51      A
ATOM   1889  CD  LYS A 234     -14.013  -5.732  59.621  1.00 82.51      A
ATOM   1890  CE  LYS A 234     -13.630  -4.794  58.484  1.00 82.51      A
ATOM   1891  NZ  LYS A 234     -14.323  -3.474  58.565  1.00 82.51      A
ATOM   1892  C   LYS A 234     -11.388  -9.128  60.761  1.00 66.11      A
ATOM   1893  O   LYS A 234     -10.661  -9.295  59.777  1.00 66.11      A
ATOM   1894  N   PHE A 235     -10.908  -8.790  61.953  1.00 53.14      A
ATOM   1895  CA  PHE A 235      -9.483  -8.541  62.132  1.00 53.14      A
ATOM   1896  CB  PHE A 235      -9.307  -7.248  62.911  1.00 56.44      A
ATOM   1897  CG  PHE A 235     -10.017  -6.085  62.295  1.00 56.44      A
ATOM   1898  CD1 PHE A 235      -9.577  -5.548  61.088  1.00 56.44      A
ATOM   1899  CD2 PHE A 235     -11.138  -5.535  62.910  1.00 56.44      A
ATOM   1900  CE1 PHE A 235     -10.242  -4.477  60.501  1.00 56.44      A
ATOM   1901  CE2 PHE A 235     -11.814  -4.465  62.333  1.00 56.44      A
ATOM   1902  CZ  PHE A 235     -11.364  -3.933  61.124  1.00 56.44      A
ATOM   1903  C   PHE A 235      -8.679  -9.651  62.792  1.00 53.14      A
ATOM   1904  O   PHE A 235      -7.457  -9.729  62.615  1.00 53.14      A
ATOM   1905  N   GLY A 236      -9.355 -10.514  63.542  1.00 55.50      A
ATOM   1906  CA  GLY A 236      -8.654 -11.589  64.223  1.00 55.50      A
ATOM   1907  C   GLY A 236      -7.992 -11.062  65.487  1.00 55.50      A
ATOM   1908  O   GLY A 236      -7.978  -9.855  65.728  1.00 55.50      A
ATOM   1909  N   GLN A 237      -7.438 -11.963  66.291  1.00 59.58      A
ATOM   1910  CA  GLN A 237      -6.780 -11.571  67.529  1.00 59.58      A
ATOM   1911  CB  GLN A 237      -6.314 -12.807  68.307  1.00100.64      A
ATOM   1912  CG  GLN A 237      -7.444 -13.720  68.767  1.00100.64      A
ATOM   1913  CD  GLN A 237      -6.986 -14.759  69.781  1.00100.64      A
ATOM   1914  OE1 GLN A 237      -6.077 -15.546  69.517  1.00100.64      A
ATOM   1915  NE2 GLN A 237      -7.620 -14.763  70.949  1.00100.64      A
ATOM   1916  C   GLN A 237      -5.592 -10.677  67.237  1.00 59.58      A
ATOM   1917  O   GLN A 237      -5.050 -10.701  66.139  1.00 59.58      A
ATOM   1918  N   VAL A 238      -5.200  -9.889  68.232  1.00 56.69      A
ATOM   1919  CA  VAL A 238      -4.069  -8.980  68.105  1.00 56.69      A
ATOM   1920  CB  VAL A 238      -3.695  -8.327  69.448  1.00 79.40      A
ATOM   1921  CG1 VAL A 238      -2.951  -7.025  69.204  1.00 79.40      A
ATOM   1922  CG2 VAL A 238      -4.919  -8.122  70.287  1.00 79.40      A
ATOM   1923  C   VAL A 238      -2.837  -9.747  67.670  1.00 56.69      A
ATOM   1924  O   VAL A 238      -2.550 -10.824  68.196  1.00 56.69      A
ATOM   1925  N   ASP A 239      -2.101  -9.190  66.719  1.00 49.95      A
ATOM   1926  CA  ASP A 239      -0.878  -9.826  66.265  1.00 49.95      A
ATOM   1927  CB  ASP A 239      -0.792  -9.814  64.737  1.00 59.63      A
ATOM   1928  CG  ASP A 239       0.354 -10.654  64.220  1.00 59.63      A
ATOM   1929  OD1 ASP A 239       0.206 -11.260  63.139  1.00 59.63      A
ATOM   1930  OD2 ASP A 239       1.406 -10.708  64.889  1.00 59.63      A
ATOM   1931  C   ASP A 239       0.226  -8.987  66.891  1.00 49.95      A
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FIGURE 25 CON'T

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ATOM   1932  O   ASP A 239       0.419  -7.826  66.531  1.00 49.95      A
ATOM   1933  N   LEU A 240       0.930  -9.579  67.850  1.00 56.76      A
ATOM   1934  CA  LEU A 240       1.983  -8.887  68.576  1.00 56.76      A
ATOM   1935  CB  LEU A 240       2.270  -9.622  69.886  1.00 64.97      A
ATOM   1936  CG  LEU A 240       1.064  -9.867  70.796  1.00 64.97      A
ATOM   1937  CD1 LEU A 240       1.507 -10.675  72.015  1.00 64.97      A
ATOM   1938  CD2 LEU A 240       0.445  -8.537  71.212  1.00 64.97      A
ATOM   1939  C   LEU A 240       3.274  -8.723  67.793  1.00 56.76      A
ATOM   1940  O   LEU A 240       4.166  -7.992  68.218  1.00 56.76      A
ATOM   1941  N   LYS A 241       3.379  -9.396  66.652  1.00 60.83      A
ATOM   1942  CA  LYS A 241       4.586  -9.289  65.843  1.00 60.83      A
ATOM   1943  CB  LYS A 241       4.756 -10.538  64.976  1.00100.72      A
ATOM   1944  CG  LYS A 241       5.042 -11.793  65.787  1.00100.72      A
ATOM   1945  CD  LYS A 241       5.175 -13.021  64.907  1.00100.72      A
ATOM   1946  CE  LYS A 241       5.448 -14.258  65.747  1.00100.72      A
ATOM   1947  NZ  LYS A 241       5.548 -15.489  64.917  1.00100.72      A

ATOM   1948  C   LYS A 241       4.594  -8.038  64.969  1.00 60.83      A
ATOM   1949  O   LYS A 241       5.624  -7.681  64.401  1.00 60.83      A
ATOM   1950  N   GLN A 242       3.449  -7.367  64.879  1.00 55.00      A
ATOM   1951  CA  GLN A 242       3.334  -6.157  64.069  1.00 55.00      A
ATOM   1952  CB  GLN A 242       1.876  -5.923  63.644  1.00 46.50      A
ATOM   1953  CG  GLN A 242       1.020  -5.292  64.737  1.00 46.50      A
ATOM   1954  CD  GLN A 242      -0.455  -5.192  64.380  1.00 46.50      A
ATOM   1955  OE1 GLN A 242      -0.872  -4.309  63.612  1.00 46.50      A
ATOM   1956  NE2 GLN A 242      -1.258  -6.097  64.936  1.00 46.50      A
ATOM   1957  C   GLN A 242       3.805  -4.934  64.841  1.00 55.00      A
ATOM   1958  O   GLN A 242       3.556  -4.809  66.038  1.00 55.00      A
ATOM   1959  N   PRO A 243       4.514  -4.021  64.170  1.00 58.47      A
ATOM   1960  CD  PRO A 243       5.203  -4.174  62.876  1.00 59.24      A
ATOM   1961  CA  PRO A 243       4.973  -2.818  64.866  1.00 58.47      A
ATOM   1962  CB  PRO A 243       6.197  -2.403  64.058  1.00 59.24      A
ATOM   1963  CG  PRO A 243       5.809  -2.802  62.670  1.00 59.24      A
ATOM   1964  C   PRO A 243       3.855  -1.779  64.787  1.00 58.47      A
ATOM   1965  O   PRO A 243       2.936  -1.922  63.979  1.00 58.47      A
ATOM   1966  N   ALA A 244       3.924  -0.749  65.623  1.00 48.59      A
ATOM   1967  CA  ALA A 244       2.917   0.302  65.603  1.00 48.59      A
ATOM   1968  CB  ALA A 244       2.690   0.851  67.008  1.00 34.86      A
ATOM   1969  C   ALA A 244       3.401   1.414  64.669  1.00 48.59      A
ATOM   1970  O   ALA A 244       4.594   1.695  64.599  1.00 48.59      A
ATOM   1971  N   ILE A 245       2.468   2.035  63.955  1.00 51.52      A
ATOM   1972  CA  ILE A 245       2.796   3.103  63.012  1.00 51.52      A
ATOM   1973  CB  ILE A 245       2.026   2.907  61.675  1.00 46.20      A
ATOM   1974  CG2 ILE A 245       2.248   4.090  60.748  1.00 46.20      A
ATOM   1975  CG1 ILE A 245       2.477   1.602  61.009  1.00 46.20      A
ATOM   1976  CD1 ILE A 245       1.664   1.232  59.792  1.00 46.20      A
ATOM   1977  C   ILE A 245       2.453   4.473  63.578  1.00 51.52      A
ATOM   1978  O   ILE A 245       1.289   4.767  63.843  1.00 51.52      A
ATOM   1979  N   LEU A 246       3.462   5.315  63.766  1.00 48.33      A
ATOM   1980  CA  LEU A 246       3.196   6.649  64.285  1.00 48.33      A
ATOM   1981  CB  LEU A 246       4.468   7.273  64.859  1.00 54.70      A
ATOM   1982  CG  LEU A 246       4.190   8.580  65.601  1.00 54.70      A
ATOM   1983  CD1 LEU A 246       3.261   8.307  66.780  1.00 54.70      A
ATOM   1984  CD2 LEU A 246       5.498   9.199  66.073  1.00 54.70      A
ATOM   1985  C   LEU A 246       2.677   7.490  63.122  1.00 48.33      A
ATOM   1986  O   LEU A 246       3.335   7.600  62.083  1.00 48.33      A
ATOM   1987  N   ALA A 247       1.500   8.080  63.287  1.00 60.06      A
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FIGURE 25 CON'T

ATOM	1988	CA	ALA	A	247	0.911	8.869	62.214	1.00	60.06	A
ATOM	1989	CB	ALA	A	247	-0.029	7.986	61.383	1.00	51.98	A
ATOM	1990	C	ALA	A	247	0.155	10.078	62.723	1.00	60.06	A
ATOM	1991	O	ALA	A	247	0.149	10.370	63.918	1.00	60.06	A
ATOM	1992	N	LYS	A	248	-0.484	10.782	61.796	1.00	56.31	A
ATOM	1993	CA	LYS	A	248	-1.265	11.960	62.126	1.00	56.31	A
ATOM	1994	CB	LYS	A	248	-0.407	13.221	61.984	1.00	104.99	A
ATOM	1995	CG	LYS	A	248	0.449	13.253	60.731	1.00	104.99	A
ATOM	1996	CD	LYS	A	248	1.273	14.536	60.631	1.00	104.99	A
ATOM	1997	CE	LYS	A	248	2.226	14.719	61.814	1.00	104.99	A
ATOM	1998	NZ	LYS	A	248	1.530	15.068	63.088	1.00	104.99	A
ATOM	1999	C	LYS	A	248	-2.482	12.039	61.216	1.00	56.31	A
ATOM	2000	O	LYS	A	248	-2.551	11.363	60.185	1.00	56.31	A
ATOM	2001	N	PHE	A	249	-3.446	12.859	61.610	1.00	63.28	A
ATOM	2002	CA	PHE	A	249	-4.661	13.030	60.838	1.00	63.28	A
ATOM	2003	CB	PHE	A	249	-5.592	14.004	61.557	1.00	78.87	A
ATOM	2004	CG	PHE	A	249	-6.051	13.511	62.897	1.00	78.87	A
ATOM	2005	CD1	PHE	A	249	-6.909	12.420	62.992	1.00	78.87	A
ATOM	2006	CD2	PHE	A	249	-5.602	14.115	64.065	1.00	78.87	A
ATOM	2007	CE1	PHE	A	249	-7.313	11.935	64.235	1.00	78.87	A
ATOM	2008	CE2	PHE	A	249	-5.999	13.639	65.314	1.00	78.87	A
ATOM	2009	CZ	PHE	A	249	-6.855	12.547	65.399	1.00	78.87	A
ATOM	2010	C	PHE	A	249	-4.350	13.534	59.436	1.00	63.28	A
ATOM	2011	O	PHE	A	249	-3.432	14.345	59.236	1.00	63.28	A
ATOM	2012	N	ALA	A	250	-5.113	13.039	58.465	1.00	68.59	A
ATOM	2013	CA	ALA	A	250	-4.935	13.438	57.078	1.00	68.59	A
ATOM	2014	CB	ALA	A	250	-5.461	12.346	56.153	1.00	55.71	A
ATOM	2015	C	ALA	A	250	-5.659	14.756	56.799	1.00	68.59	A
ATOM	2016	O	ALA	A	250	-5.209	15.562	55.982	1.00	68.59	A
ATOM	2017	N	SER	A	251	-6.772	14.972	57.493	1.00	76.45	A
ATOM	2018	CA	SER	A	251	-7.582	16.175	57.317	1.00	76.45	A
ATOM	2019	CB	SER	A	251	-8.890	16.032	58.099	1.00	150.67	A
ATOM	2020	OG	SER	A	251	-8.635	15.831	59.480	1.00	150.67	A
ATOM	2021	C	SER	A	251	-6.890	17.480	57.722	1.00	76.45	A
ATOM	2022	O	SER	A	251	-5.672	17.616	57.598	1.00	76.45	A
ATOM	2023	N	LYS	A	252	-7.688	18.432	58.204	1.00	116.94	A
ATOM	2024	CA	LYS	A	252	-7.206	19.746	58.626	1.00	116.94	A
ATOM	2025	CB	LYS	A	252	-5.914	19.623	59.445	1.00	124.94	A
ATOM	2026	CG	LYS	A	252	-6.066	18.863	60.753	1.00	124.94	A
ATOM	2027	CD	LYS	A	252	-4.724	18.721	61.457	1.00	124.94	A
ATOM	2028	CE	LYS	A	252	-4.853	17.950	62.763	1.00	124.94	A
ATOM	2029	NZ	LYS	A	252	-5.732	18.647	63.743	1.00	124.94	A
ATOM	2030	C	LYS	A	252	-6.957	20.629	57.409	1.00	116.94	A
ATOM	2031	O	LYS	A	252	-7.464	20.356	56.320	1.00	116.94	A
ATOM	2032	N	ASN	A	258	1.361	17.852	65.655	1.00	150.47	A
ATOM	2033	CA	ASN	A	258	0.210	18.540	66.229	1.00	150.47	A
ATOM	2034	CB	ASN	A	258	-0.659	19.139	65.116	1.00	149.86	A
ATOM	2035	CG	ASN	A	258	-1.774	20.029	65.651	1.00	149.86	A
ATOM	2036	OD1	ASN	A	258	-2.656	20.452	64.903	1.00	149.86	A
ATOM	2037	ND2	ASN	A	258	-1.732	20.324	66.946	1.00	149.86	A
ATOM	2038	C	ASN	A	258	-0.627	17.576	67.064	1.00	150.47	A
ATOM	2039	O	ASN	A	258	-1.557	17.989	67.758	1.00	150.47	A
ATOM	2040	N	TYR	A	259	-0.294	16.290	66.999	1.00	138.22	A
ATOM	2041	CA	TYR	A	259	-1.036	15.289	67.755	1.00	138.22	A
ATOM	2042	CB	TYR	A	259	-2.447	15.151	67.181	1.00	99.01	A
ATOM	2043	CG	TYR	A	259	-3.458	14.566	68.141	1.00	99.01	A
ATOM	2044	CD1	TYR	A	259	-3.942	15.311	69.216	1.00	99.01	A

ATOM	2045	CE1	TYR	A	259	-4.893	14.783	70.089	1.00	99.01	A
ATOM	2046	CD2	TYR	A	259	-3.948	13.274	67.965	1.00	99.01	A
ATOM	2047	CE2	TYR	A	259	-4.897	12.737	68.829	1.00	99.01	A
ATOM	2048	CZ	TYR	A	259	-5.366	13.496	69.886	1.00	99.01	A
ATOM	2049	OH	TYR	A	259	-6.314	12.968	70.732	1.00	99.01	A
ATOM	2050	C	TYR	A	259	-0.344	13.928	67.734	1.00	138.22	A
ATOM	2051	O	TYR	A	259	0.060	13.410	68.776	1.00	138.22	A
ATOM	2052	N	LYS	A	260	-0.215	13.355	66.540	1.00	83.39	A
ATOM	2053	CA	LYS	A	260	0.415	12.048	66.362	1.00	83.39	A
ATOM	2054	CB	LYS	A	260	1.852	12.061	66.897	1.00	85.61	A
ATOM	2055	CG	LYS	A	260	2.822	12.856	66.033	1.00	85.61	A
ATOM	2056	CD	LYS	A	260	4.250	12.788	66.563	1.00	85.61	A
ATOM	2057	CE	LYS	A	260	4.365	13.409	67.946	1.00	85.61	A
ATOM	2058	NZ	LYS	A	260	3.853	14.806	67.967	1.00	85.61	A
ATOM	2059	C	LYS	A	260	-0.374	10.914	67.016	1.00	83.39	A
ATOM	2060	O	LYS	A	260	-0.565	10.884	68.231	1.00	83.39	A
ATOM	2061	N	ILE	A	261	-0.829	9.985	66.184	1.00	62.77	A
ATOM	2062	CA	ILE	A	261	-1.608	8.831	66.621	1.00	62.77	A
ATOM	2063	CB	ILE	A	261	-3.003	8.802	65.923	1.00	58.19	A
ATOM	2064	CG2	ILE	A	261	-3.803	7.598	66.380	1.00	58.19	A
ATOM	2065	CG1	ILE	A	261	-3.774	10.091	66.227	1.00	58.19	A
ATOM	2066	CD1	ILE	A	261	-3.252	11.311	65.498	1.00	58.19	A
ATOM	2067	C	ILE	A	261	-0.863	7.550	66.251	1.00	62.77	A
ATOM	2068	O	ILE	A	261	-0.047	7.541	65.328	1.00	62.77	A
ATOM	2069	N	TYR	A	262	-1.141	6.475	66.981	1.00	45.49	A
ATOM	2070	CA	TYR	A	262	-0.529	5.178	66.715	1.00	45.49	A
ATOM	2071	CB	TYR	A	262	-0.166	4.465	68.019	1.00	68.83	A
ATOM	2072	CG	TYR	A	262	1.284	4.622	68.423	1.00	68.83	A
ATOM	2073	CD1	TYR	A	262	2.311	4.218	67.571	1.00	68.83	A
ATOM	2074	CE1	TYR	A	262	3.647	4.353	67.939	1.00	68.83	A
ATOM	2075	CD2	TYR	A	262	1.630	5.167	69.656	1.00	68.83	A
ATOM	2076	CE2	TYR	A	262	2.959	5.306	70.035	1.00	68.83	A
ATOM	2077	CZ	TYR	A	262	3.964	4.897	69.174	1.00	68.83	A
ATOM	2078	OH	TYR	A	262	5.284	5.034	69.546	1.00	68.83	A
ATOM	2079	C	TYR	A	262	-1.541	4.342	65.948	1.00	45.49	A
ATOM	2080	O	TYR	A	262	-2.726	4.297	66.309	1.00	45.49	A
ATOM	2081	N	LEU	A	263	-1.076	3.687	64.888	1.00	40.09	A
ATOM	2082	CA	LEU	A	263	-1.948	2.853	64.070	1.00	40.09	A
ATOM	2083	CB	LEU	A	263	-2.014	3.393	62.633	1.00	50.45	A
ATOM	2084	CG	LEU	A	263	-2.482	4.837	62.440	1.00	50.45	A
ATOM	2085	CD1	LEU	A	263	-2.321	5.233	60.970	1.00	50.45	A
ATOM	2086	CD2	LEU	A	263	-3.929	4.974	62.901	1.00	50.45	A
ATOM	2087	C	LEU	A	263	-1.441	1.423	64.025	1.00	40.09	A
ATOM	2088	O	LEU	A	263	-0.236	1.172	64.097	1.00	40.09	A
ATOM	2089	N	LEU	A	264	-2.369	0.486	63.903	1.00	45.51	A
ATOM	2090	CA	LEU	A	264	-2.017	-0.921	63.809	1.00	45.51	A
ATOM	2091	CB	LEU	A	264	-2.868	-1.752	64.772	1.00	44.81	A
ATOM	2092	CG	LEU	A	264	-2.442	-1.822	66.245	1.00	44.81	A
ATOM	2093	CD1	LEU	A	264	-2.185	-0.438	66.816	1.00	44.81	A
ATOM	2094	CD2	LEU	A	264	-3.531	-2.534	67.030	1.00	44.81	A
ATOM	2095	C	LEU	A	264	-2.271	-1.373	62.364	1.00	45.51	A
ATOM	2096	O	LEU	A	264	-3.409	-1.350	61.896	1.00	45.51	A
ATOM	2097	N	PRO	A	265	-1.206	-1.766	61.639	1.00	47.17	A
ATOM	2098	CD	PRO	A	265	0.196	-1.780	62.082	1.00	53.05	A
ATOM	2099	CA	PRO	A	265	-1.309	-2.223	60.249	1.00	47.17	A
ATOM	2100	CB	PRO	A	265	0.105	-2.733	59.935	1.00	53.05	A

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ATOM	2101	CG	PRO	A	265	0.752	-2.908	61.273	1.00	53.05	A
ATOM	2102	C	PRO	A	265	-2.375	-3.289	60.054	1.00	47.17	A
ATOM	2103	O	PRO	A	265	-2.897	-3.482	58.951	1.00	47.17	A
ATOM	2104	N	GLN	A	266	-2.705	-3.954	61.154	1.00	44.41	A
ATOM	2105	CA	GLN	A	266	-3.703	-5.014	61.188	1.00	44.41	A
ATOM	2106	CB	GLN	A	266	-3.555	-5.805	62.500	1.00	52.67	A
ATOM	2107	CG	GLN	A	266	-4.446	-7.029	62.628	1.00	52.67	A
ATOM	2108	CD	GLN	A	266	-4.397	-7.640	64.026	1.00	52.67	A
ATOM	2109	OE1	GLN	A	266	-3.465	-7.390	64.789	1.00	52.67	A
ATOM	2110	NE2	GLN	A	266	-5.399	-8.453	64.361	1.00	52.67	A
ATOM	2111	C	GLN	A	266	-5.109	-4.439	61.111	1.00	44.41	A
ATOM	2112	O	GLN	A	266	-6.053	-5.141	60.757	1.00	44.41	A
ATOM	2113	N	LEU	A	267	-5.243	-3.162	61.449	1.00	42.63	A
ATOM	2114	CA	LEU	A	267	-6.548	-2.518	61.459	1.00	42.63	A
ATOM	2115	CB	LEU	A	267	-6.815	-1.935	62.851	1.00	46.28	A
ATOM	2116	CG	LEU	A	267	-6.670	-2.853	64.069	1.00	46.28	A
ATOM	2117	CD1	LEU	A	267	-6.996	-2.057	65.324	1.00	46.28	A
ATOM	2118	CD2	LEU	A	267	-7.597	-4.056	63.942	1.00	46.28	A
ATOM	2119	C	LEU	A	267	-6.749	-1.411	60.430	1.00	42.63	A
ATOM	2120	O	LEU	A	267	-7.811	-0.782	60.403	1.00	42.63	A
ATOM	2121	N	VAL	A	268	-5.743	-1.154	59.599	1.00	50.36	A
ATOM	2122	CA	VAL	A	268	-5.853	-0.092	58.605	1.00	50.36	A
ATOM	2123	CB	VAL	A	268	-4.875	1.049	58.898	1.00	36.71	A
ATOM	2124	CG1	VAL	A	268	-5.222	1.693	60.228	1.00	36.71	A
ATOM	2125	CG2	VAL	A	268	-3.425	0.520	58.869	1.00	36.71	A
ATOM	2126	C	VAL	A	268	-5.605	-0.532	57.171	1.00	50.36	A
ATOM	2127	O	VAL	A	268	-4.858	-1.474	56.908	1.00	50.36	A
ATOM	2128	N	VAL	A	269	-6.227	0.177	56.239	1.00	41.89	A
ATOM	2129	CA	VAL	A	269	-6.054	-0.144	54.834	1.00	41.89	A
ATOM	2130	CB	VAL	A	269	-7.389	-0.501	54.162	1.00	36.78	A
ATOM	2131	CG1	VAL	A	269	-8.045	-1.675	54.879	1.00	36.78	A
ATOM	2132	CG2	VAL	A	269	-8.293	0.711	54.150	1.00	36.78	A
ATOM	2133	C	VAL	A	269	-5.463	1.028	54.071	1.00	41.89	A
ATOM	2134	O	VAL	A	269	-5.777	2.186	54.345	1.00	41.89	A
ATOM	2135	N	PRO	A	270	-4.566	0.738	53.125	1.00	45.86	A
ATOM	2136	CD	PRO	A	270	-3.742	-0.476	53.021	1.00	42.86	A
ATOM	2137	CA	PRO	A	270	-3.989	1.841	52.359	1.00	45.86	A
ATOM	2138	CB	PRO	A	270	-2.840	1.180	51.579	1.00	42.86	A
ATOM	2139	CG	PRO	A	270	-3.074	-0.279	51.704	1.00	42.86	A
ATOM	2140	C	PRO	A	270	-5.063	2.467	51.458	1.00	45.86	A
ATOM	2141	O	PRO	A	270	-5.921	1.766	50.914	1.00	45.86	A
ATOM	2142	N	THR	A	271	-5.027	3.790	51.341	1.00	47.94	A
ATOM	2143	CA	THR	A	271	-5.987	4.526	50.524	1.00	47.94	A
ATOM	2144	CB	THR	A	271	-7.025	5.267	51.381	1.00	76.25	A
ATOM	2145	OG1	THR	A	271	-7.294	4.516	52.570	1.00	76.25	A
ATOM	2146	CG2	THR	A	271	-8.316	5.439	50.601	1.00	76.25	A
ATOM	2147	C	THR	A	271	-5.224	5.570	49.731	1.00	47.94	A
ATOM	2148	O	THR	A	271	-4.190	6.065	50.186	1.00	47.94	A
ATOM	2149	N	TYR	A	272	-5.750	5.918	48.561	1.00	43.35	A
ATOM	2150	CA	TYR	A	272	-5.112	6.890	47.676	1.00	43.35	A
ATOM	2151	CB	TYR	A	272	-4.320	6.167	46.583	1.00	43.00	A
ATOM	2152	CG	TYR	A	272	-3.239	5.233	47.053	1.00	43.00	A
ATOM	2153	CD1	TYR	A	272	-1.992	5.722	47.442	1.00	43.00	A
ATOM	2154	CE1	TYR	A	272	-0.987	4.868	47.855	1.00	43.00	A
ATOM	2155	CD2	TYR	A	272	-3.454	3.855	47.091	1.00	43.00	A
ATOM	2156	CE2	TYR	A	272	-2.453	2.984	47.502	1.00	43.00	A
ATOM	2157	CZ	TYR	A	272	-1.222	3.498	47.883	1.00	43.00	A

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ATOM	2158	OH	TYR	A	272	-0.222	2.652	48.291	1.00	43.00	A
ATOM	2159	C	TYR	A	272	-6.130	7.769	46.956	1.00	43.35	A
ATOM	2160	O	TYR	A	272	-7.227	7.311	46.620	1.00	43.35	A
ATOM	2161	N	ASN	A	273	-5.764	9.029	46.728	1.00	37.52	A
ATOM	2162	CA	ASN	A	273	-6.613	9.929	45.948	1.00	37.52	A
ATOM	2163	CB	ASN	A	273	-6.359	11.398	46.300	1.00	68.70	A
ATOM	2164	CG	ASN	A	273	-6.931	11.774	47.656	1.00	68.70	A
ATOM	2165	OD1	ASN	A	273	-8.059	11.400	47.989	1.00	68.70	A
ATOM	2166	ND2	ASN	A	273	-6.158	12.521	48.445	1.00	68.70	A
ATOM	2167	C	ASN	A	273	-6.136	9.629	44.527	1.00	37.52	A
ATOM	2168	O	ASN	A	273	-4.990	9.922	44.175	1.00	37.52	A
ATOM	2169	N	ALA	A	274	-6.988	9.002	43.728	1.00	38.51	A
ATOM	2170	CA	ALA	A	274	-6.609	8.629	42.359	1.00	38.51	A
ATOM	2171	CB	ALA	A	274	-7.815	8.069	41.615	1.00	48.04	A
ATOM	2172	C	ALA	A	274	-6.013	9.782	41.565	1.00	38.51	A
ATOM	2173	O	ALA	A	274	-4.946	9.649	40.966	1.00	38.51	A
ATOM	2174	N	GLU	A	275	-6.706	10.915	41.580	1.00	46.05	A
ATOM	2175	CA	GLU	A	275	-6.279	12.098	40.846	1.00	46.05	A
ATOM	2176	CB	GLU	A	275	-7.351	13.193	40.948	1.00	49.75	A
ATOM	2177	CG	GLU	A	275	-8.585	13.001	40.029	1.00	49.75	A
ATOM	2178	CD	GLU	A	275	-9.477	11.819	40.403	1.00	49.75	A
ATOM	2179	OE1	GLU	A	275	-9.694	11.589	41.609	1.00	49.75	A
ATOM	2180	OE2	GLU	A	275	-9.982	11.128	39.485	1.00	49.75	A
ATOM	2181	C	GLU	A	275	-4.928	12.654	41.299	1.00	46.05	A
ATOM	2182	O	GLU	A	275	-4.297	13.422	40.580	1.00	46.05	A
ATOM	2183	N	GLN	A	276	-4.487	12.256	42.486	1.00	62.96	A
ATOM	2184	CA	GLN	A	276	-3.215	12.717	43.036	1.00	62.96	A
ATOM	2185	CB	GLN	A	276	-3.300	12.738	44.566	1.00	90.77	A
ATOM	2186	CG	GLN	A	276	-2.027	13.162	45.274	1.00	90.77	A
ATOM	2187	CD	GLN	A	276	-2.101	12.943	46.775	1.00	90.77	A
ATOM	2188	OE1	GLN	A	276	-2.984	13.477	47.449	1.00	90.77	A
ATOM	2189	NE2	GLN	A	276	-1.173	12.149	47.305	1.00	90.77	A
ATOM	2190	C	GLN	A	276	-2.036	11.844	42.601	1.00	62.96	A
ATOM	2191	O	GLN	A	276	-0.881	12.209	42.804	1.00	62.96	A
ATOM	2192	N	LEU	A	277	-2.326	10.693	42.005	1.00	55.21	A
ATOM	2193	CA	LEU	A	277	-1.271	9.786	41.568	1.00	55.21	A
ATOM	2194	CB	LEU	A	277	-1.759	8.337	41.656	1.00	51.32	A
ATOM	2195	CG	LEU	A	277	-2.321	7.937	43.025	1.00	51.32	A
ATOM	2196	CD1	LEU	A	277	-2.811	6.487	42.999	1.00	51.32	A
ATOM	2197	CD2	LEU	A	277	-1.247	8.132	44.082	1.00	51.32	A
ATOM	2198	C	LEU	A	277	-0.823	10.093	40.140	1.00	55.21	A
ATOM	2199	O	LEU	A	277	-1.622	10.554	39.317	1.00	55.21	A
ATOM	2200	N	ALA	A	282	-2.259	2.294	38.184	1.00	112.07	A
ATOM	2201	CA	ALA	A	282	-1.574	1.210	37.496	1.00	112.07	A
ATOM	2202	CB	ALA	A	282	-2.064	-0.138	38.011	1.00	57.82	A
ATOM	2203	C	ALA	A	282	-1.805	1.306	36.000	1.00	112.07	A
ATOM	2204	O	ALA	A	282	-1.167	2.102	35.316	1.00	112.07	A
ATOM	2205	N	LYS	A	283	-2.730	0.502	35.491	1.00	65.34	A
ATOM	2206	CA	LYS	A	283	-3.013	0.506	34.061	1.00	65.34	A
ATOM	2207	CB	LYS	A	283	-2.276	-0.663	33.389	1.00	114.62	A
ATOM	2208	CG	LYS	A	283	-0.953	-1.023	34.079	1.00	114.62	A
ATOM	2209	CD	LYS	A	283	0.197	-1.284	33.104	1.00	114.62	A
ATOM	2210	CE	LYS	A	283	0.076	-2.626	32.395	1.00	114.62	A
ATOM	2211	NZ	LYS	A	283	-1.071	-2.674	31.451	1.00	114.62	A
ATOM	2212	C	LYS	A	283	-4.515	0.376	33.860	1.00	65.34	A
ATOM	2213	O	LYS	A	283	-5.162	1.247	33.273	1.00	65.34	A

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ATOM   2214  N   GLU A 284     -5.055  -0.729  34.360  1.00 67.78      A
ATOM   2215  CA  GLU A 284     -6.475  -1.019  34.291  1.00 67.78      A
ATOM   2216  CB  GLU A 284     -6.741  -2.436  34.795  1.00154.43      A
ATOM   2217  CG  GLU A 284     -6.135  -3.521  33.929  1.00154.43      A
ATOM   2218  CD  GLU A 284     -5.826  -4.777  34.713  1.00154.43      A
ATOM   2219  OE1 GLU A 284     -4.972  -4.706  35.622  1.00154.43      A
ATOM   2220  OE2 GLU A 284     -6.434  -5.830  34.425  1.00154.43      A
ATOM   2221  C   GLU A 284     -7.202  -0.020  35.172  1.00 67.78      A
ATOM   2222  O   GLU A 284     -8.275   0.468  34.812  1.00 67.78      A
ATOM   2223  N   ILE A 285     -6.621   0.281  36.333  1.00 59.11      A
ATOM   2224  CA  ILE A 285     -7.244   1.243  37.233  1.00 59.11      A
ATOM   2225  CB  ILE A 285     -6.463   1.414  38.555  1.00 56.69      A
ATOM   2226  CG2 ILE A 285     -6.974   2.657  39.305  1.00 56.69      A
ATOM   2227  CG1 ILE A 285     -6.629   0.165  39.420  1.00 56.69      A
ATOM   2228  CD1 ILE A 285     -5.905   0.227  40.746  1.00 56.69      A
ATOM   2229  C   ILE A 285     -7.296   2.588  36.538  1.00 59.11      A
ATOM   2230  O   ILE A 285     -8.374   3.134  36.295  1.00 59.11      A
ATOM   2231  N   LEU A 286     -6.117   3.108  36.212  1.00 87.11      A
ATOM   2232  CA  LEU A 286     -5.993   4.393  35.541  1.00 87.11      A
ATOM   2233  CB  LEU A 286     -4.648   4.482  34.821  1.00 84.12      A
ATOM   2234  CG  LEU A 286     -4.369   5.809  34.112  1.00 84.12      A
ATOM   2235  CD1 LEU A 286     -4.314   6.926  35.149  1.00 84.12      A
ATOM   2236  CD2 LEU A 286     -3.063   5.726  33.331  1.00 84.12      A
ATOM   2237  C   LEU A 286     -7.119   4.599  34.540  1.00 87.11      A
ATOM   2238  O   LEU A 286     -7.734   5.659  34.499  1.00 87.11      A
ATOM   2239  N   GLU A 287     -7.387   3.581  33.734  1.00 74.75      A
ATOM   2240  CA  GLU A 287     -8.442   3.664  32.739  1.00 74.75      A
ATOM   2241  CB  GLU A 287     -8.646   2.308  32.058  1.00118.41      A
ATOM   2242  CG  GLU A 287     -7.445   1.801  31.278  1.00118.41      A
ATOM   2243  CD  GLU A 287     -7.669   0.416  30.691  1.00118.41      A
ATOM   2244  OE1 GLU A 287     -6.762  -0.090  29.997  1.00118.41      A
ATOM   2245  OE2 GLU A 287     -8.750  -0.167  30.926  1.00118.41      A
ATOM   2246  C   GLU A 287     -9.748   4.089  33.393  1.00 74.75      A
ATOM   2247  O   GLU A 287    -10.250   5.183  33.143  1.00 74.75      A
ATOM   2248  N   TYR A 288    -10.277   3.218  34.247  1.00 53.07      A
ATOM   2249  CA  TYR A 288    -11.540   3.443  34.938  1.00 53.07      A
ATOM   2250  CB  TYR A 288    -11.732   2.396  36.047  1.00 53.22      A
ATOM   2251  CG  TYR A 288    -13.171   2.281  36.487  1.00 53.22      A
ATOM   2252  CD1 TYR A 288    -14.131   1.767  35.622  1.00 53.22      A
ATOM   2253  CE1 TYR A 288    -15.470   1.722  35.972  1.00 53.22      A
ATOM   2254  CD2 TYR A 288    -13.588   2.747  37.733  1.00 53.22      A
ATOM   2255  CE2 TYR A 288    -14.940   2.707  38.100  1.00 53.22      A
ATOM   2256  CZ  TYR A 288    -15.873   2.194  37.205  1.00 53.22      A
ATOM   2257  OH  TYR A 288    -17.218   2.171  37.516  1.00 53.22      A
ATOM   2258  C   TYR A 288    -11.736   4.834  35.533  1.00 53.07      A
ATOM   2259  O   TYR A 288    -12.866   5.315  35.628  1.00 53.07      A
ATOM   2260  N   THR A 289    -10.645   5.471  35.947  1.00 51.30      A
ATOM   2261  CA  THR A 289    -10.723   6.801  36.542  1.00 51.30      A
ATOM   2262  CB  THR A 289     -9.546   7.052  37.477  1.00 45.40      A
ATOM   2263  OG1 THR A 289     -8.329   6.831  36.759  1.00 45.40      A
ATOM   2264  CG2 THR A 289     -9.606   6.119  38.679  1.00 45.40      A
ATOM   2265  C   THR A 289    -10.732   7.901  35.489  1.00 51.30      A
ATOM   2266  O   THR A 289    -11.073   9.047  35.774  1.00 51.30      A
ATOM   2267  N   LYS A 290    -10.346   7.563  34.269  1.00 45.85      A
ATOM   2268  CA  LYS A 290    -10.338   8.555  33.211  1.00 45.85      A
ATOM   2269  CB  LYS A 290     -9.221   8.260  32.210  1.00 58.48      A
ATOM   2270  CG  LYS A 290     -7.825   8.280  32.843  1.00 58.48      A
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ATOM	2271	CD	LYS	A	290	-7.517	9.621	33.528	1.00	58.48	A
ATOM	2272	CE	LYS	A	290	-7.372	10.758	32.508	1.00	58.48	A
ATOM	2273	NZ	LYS	A	290	-7.339	12.131	33.106	1.00	58.48	A
ATOM	2274	C	LYS	A	290	-11.709	8.544	32.547	1.00	45.85	A
ATOM	2275	O	LYS	A	290	-12.184	7.509	32.082	1.00	45.85	A
ATOM	2276	N	LEU	A	291	-12.354	9.701	32.546	1.00	45.06	A
ATOM	2277	CA	LEU	A	291	-13.677	9.843	31.973	1.00	45.06	A
ATOM	2278	CB	LEU	A	291	-14.662	10.308	33.056	1.00	38.73	A
ATOM	2279	CG	LEU	A	291	-14.897	9.348	34.231	1.00	38.73	A
ATOM	2280	CD1	LEU	A	291	-15.715	10.018	35.319	1.00	38.73	A
ATOM	2281	CD2	LEU	A	291	-15.621	8.082	33.715	1.00	38.73	A
ATOM	2282	C	LEU	A	291	-13.659	10.847	30.831	1.00	45.06	A
ATOM	2283	O	LEU	A	291	-13.199	11.979	30.988	1.00	45.06	A
ATOM	2284	N	MSE	A	292	-14.160	10.427	29.679	1.00	39.88	A
ATOM	2285	CA	MSE	A	292	-14.232	11.300	28.512	1.00	39.88	A
ATOM	2286	CB	MSE	A	292	-14.791	10.531	27.310	1.00	87.18	A
ATOM	2287	CG	MSE	A	292	-13.928	9.368	26.842	1.00	87.18	A
ATOM	2288	SE	MSE	A	292	-12.260	9.931	26.037	1.00	87.18	A
ATOM	2289	CE	MSE	A	292	-12.831	9.966	24.187	1.00	87.18	A
ATOM	2290	C	MSE	A	292	-15.155	12.469	28.847	1.00	39.88	A
ATOM	2291	O	MSE	A	292	-16.013	12.360	29.726	1.00	39.88	A
ATOM	2292	N	PRO	A	293	-14.985	13.607	28.156	1.00	44.59	A
ATOM	2293	CD	PRO	A	293	-13.958	13.862	27.127	1.00	38.08	A
ATOM	2294	CA	PRO	A	293	-15.814	14.794	28.383	1.00	44.59	A
ATOM	2295	CB	PRO	A	293	-15.418	15.716	27.232	1.00	38.08	A
ATOM	2296	CG	PRO	A	293	-13.959	15.360	27.019	1.00	38.08	A
ATOM	2297	C	PRO	A	293	-17.315	14.488	28.378	1.00	44.59	A
ATOM	2298	O	PRO	A	293	-18.063	15.006	29.210	1.00	44.59	A
ATOM	2299	N	GLU	A	294	-17.760	13.645	27.447	1.00	39.36	A
ATOM	2300	CA	GLU	A	294	-19.186	13.319	27.361	1.00	39.36	A
ATOM	2301	CB	GLU	A	294	-19.519	12.704	25.996	1.00	76.95	A
ATOM	2302	CG	GLU	A	294	-19.579	13.729	24.856	1.00	76.95	A
ATOM	2303	CD	GLU	A	294	-20.615	14.834	25.093	1.00	76.95	A
ATOM	2304	OE1	GLU	A	294	-21.799	14.502	25.329	1.00	76.95	A
ATOM	2305	OE2	GLU	A	294	-20.250	16.034	25.039	1.00	76.95	A
ATOM	2306	C	GLU	A	294	-19.678	12.410	28.490	1.00	39.36	A
ATOM	2307	O	GLU	A	294	-20.839	12.477	28.880	1.00	39.36	A
ATOM	2308	N	GLU	A	295	-18.798	11.561	29.007	1.00	41.51	A
ATOM	2309	CA	GLU	A	295	-19.165	10.679	30.110	1.00	41.51	A
ATOM	2310	CB	GLU	A	295	-18.082	9.620	30.302	1.00	56.10	A
ATOM	2311	CG	GLU	A	295	-17.764	8.902	29.009	1.00	56.10	A
ATOM	2312	CD	GLU	A	295	-16.696	7.842	29.159	1.00	56.10	A
ATOM	2313	OE1	GLU	A	295	-15.576	8.164	29.619	1.00	56.10	A
ATOM	2314	OE2	GLU	A	295	-16.982	6.683	28.804	1.00	56.10	A
ATOM	2315	C	GLU	A	295	-19.377	11.489	31.399	1.00	41.51	A
ATOM	2316	O	GLU	A	295	-20.358	11.295	32.114	1.00	41.51	A
ATOM	2317	N	ARG	A	296	-18.460	12.400	31.694	1.00	38.96	A
ATOM	2318	CA	ARG	A	296	-18.592	13.237	32.885	1.00	38.96	A
ATOM	2319	CB	ARG	A	296	-17.385	14.189	33.025	1.00	33.95	A
ATOM	2320	CG	ARG	A	296	-16.105	13.523	33.582	1.00	33.95	A
ATOM	2321	CD	ARG	A	296	-14.897	14.502	33.609	1.00	33.95	A
ATOM	2322	NE	ARG	A	296	-13.694	13.815	34.068	1.00	33.95	A
ATOM	2323	CZ	ARG	A	296	-13.390	13.605	35.352	1.00	33.95	A
ATOM	2324	NH1	ARG	A	296	-14.200	14.050	36.307	1.00	33.95	A
ATOM	2325	NH2	ARG	A	296	-12.296	12.908	35.680	1.00	33.95	A
ATOM	2326	C	ARG	A	296	-19.871	14.049	32.755	1.00	38.96	A
ATOM	2327	O	ARG	A	296	-20.634	14.170	33.707	1.00	38.96	A

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ATOM   2328  N   LYS A 297     -20.103  14.592  31.560  1.00 39.66      A
ATOM   2329  CA  LYS A 297     -21.286  15.408  31.300  1.00 39.66      A
ATOM   2330  CB  LYS A 297     -21.295  15.865  29.843  1.00 56.25      A
ATOM   2331  CG  LYS A 297     -22.431  16.814  29.479  1.00 56.25      A

ATOM   2332  CD  LYS A 297     -22.351  17.214  28.003  1.00 56.25      A
ATOM   2333  CE  LYS A 297     -23.438  18.198  27.634  1.00 56.25      A
ATOM   2334  NZ  LYS A 297     -24.802  17.627  27.845  1.00 56.25      A
ATOM   2335  C   LYS A 297     -22.563  14.629  31.607  1.00 39.66      A
ATOM   2336  O   LYS A 297     -23.444  15.103  32.340  1.00 39.66      A
ATOM   2337  N   GLU A 298     -22.651  13.430  31.042  1.00 40.20      A
ATOM   2338  CA  GLU A 298     -23.804  12.568  31.254  1.00 40.20      A
ATOM   2339  CB  GLU A 298     -23.665  11.314  30.397  1.00 70.61      A
ATOM   2340  CG  GLU A 298     -24.824  10.362  30.519  1.00 70.61      A
ATOM   2341  CD  GLU A 298     -24.775   9.264  29.482  1.00 70.61      A
ATOM   2342  OE1 GLU A 298     -25.751   8.494  29.398  1.00 70.61      A
ATOM   2343  OE2 GLU A 298     -23.764   9.168  28.750  1.00 70.61      A
ATOM   2344  C   GLU A 298     -23.965  12.169  32.727  1.00 40.20      A
ATOM   2345  O   GLU A 298     -25.065  12.244  33.274  1.00 40.20      A
ATOM   2346  N   LEU A 299     -22.878  11.731  33.366  1.00 39.60      A
ATOM   2347  CA  LEU A 299     -22.956  11.335  34.777  1.00 39.60      A
ATOM   2348  CB  LEU A 299     -21.585  10.868  35.284  1.00 34.67      A
ATOM   2349  CG  LEU A 299     -21.077   9.550  34.673  1.00 34.67      A
ATOM   2350  CD1 LEU A 299     -19.663   9.229  35.180  1.00 34.67      A
ATOM   2351  CD2 LEU A 299     -22.030   8.405  35.053  1.00 34.67      A
ATOM   2352  C   LEU A 299     -23.480  12.502  35.618  1.00 39.60      A
ATOM   2353  O   LEU A 299     -24.340  12.329  36.470  1.00 39.60      A
ATOM   2354  N   LEU A 300     -22.978  13.702  35.369  1.00 38.08      A
ATOM   2355  CA  LEU A 300     -23.459  14.858  36.117  1.00 38.08      A
ATOM   2356  CB  LEU A 300     -22.655  16.105  35.754  1.00 35.05      A
ATOM   2357  CG  LEU A 300     -21.217  16.121  36.295  1.00 35.05      A
ATOM   2358  CD1 LEU A 300     -20.608  17.488  35.994  1.00 35.05      A
ATOM   2359  CD2 LEU A 300     -21.214  15.844  37.820  1.00 35.05      A
ATOM   2360  C   LEU A 300     -24.950  15.106  35.852  1.00 38.08      A
ATOM   2361  O   LEU A 300     -25.715  15.422  36.775  1.00 38.08      A
ATOM   2362  N   GLU A 301     -25.364  14.979  34.595  1.00 40.84      A
ATOM   2363  CA  GLU A 301     -26.778  15.167  34.281  1.00 40.84      A
ATOM   2364  CB  GLU A 301     -27.013  15.099  32.764  1.00 49.55      A
ATOM   2365  CG  GLU A 301     -26.327  16.239  32.044  1.00 49.55      A
ATOM   2366  CD  GLU A 301     -26.457  16.181  30.544  1.00 49.55      A
ATOM   2367  OE1 GLU A 301     -26.651  15.075  29.996  1.00 49.55      A
ATOM   2368  OE2 GLU A 301     -26.344  17.251  29.912  1.00 49.55      A
ATOM   2369  C   GLU A 301     -27.615  14.108  35.002  1.00 40.84      A
ATOM   2370  O   GLU A 301     -28.724  14.391  35.418  1.00 40.84      A
ATOM   2371  N   ASN A 302     -27.075  12.900  35.164  1.00 46.53      A
ATOM   2372  CA  ASN A 302     -27.805  11.837  35.854  1.00 46.53      A
ATOM   2373  CB  ASN A 302     -27.052  10.513  35.784  1.00 44.80      A
ATOM   2374  CG  ASN A 302     -26.999   9.953  34.389  1.00 44.80      A
ATOM   2375  OD1 ASN A 302     -27.938  10.124  33.604  1.00 44.80      A
ATOM   2376  ND2 ASN A 302     -25.911   9.265  34.069  1.00 44.80      A
ATOM   2377  C   ASN A 302     -28.015  12.189  37.313  1.00 46.53      A
ATOM   2378  O   ASN A 302     -29.085  11.950  37.880  1.00 46.53      A
ATOM   2379  N   ILE A 303     -26.975  12.746  37.923  1.00 45.54      A
ATOM   2380  CA  ILE A 303     -27.036  13.141  39.319  1.00 45.54      A
ATOM   2381  CB  ILE A 303     -25.650  13.646  39.823  1.00 31.97      A
ATOM   2382  CG2 ILE A 303     -25.800  14.265  41.202  1.00 31.97      A
ATOM   2383  CG1 ILE A 303     -24.647  12.477  39.806  1.00 31.97      A
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FIGURE 25 CON'T
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ATOM	2384	CD1	ILE	A	303	-23.167	12.888	39.983	1.00	31.97	A
ATOM	2385	C	ILE	A	303	-28.056	14.250	39.467	1.00	45.54	A
ATOM	2386	O	ILE	A	303	-28.868	14.246	40.398	1.00	45.54	A
ATOM	2387	N	LEU	A	304	-28.014	15.198	38.539	1.00	47.06	A
ATOM	2388	CA	LEU	A	304	-28.928	16.325	38.571	1.00	47.06	A
ATOM	2389	CB	LEU	A	304	-28.582	17.325	37.467	1.00	43.97	A
ATOM	2390	CG	LEU	A	304	-27.253	18.080	37.610	1.00	43.97	A
ATOM	2391	CD1	LEU	A	304	-27.047	19.001	36.400	1.00	43.97	A
ATOM	2392	CD2	LEU	A	304	-27.261	18.882	38.916	1.00	43.97	A
ATOM	2393	C	LEU	A	304	-30.383	15.881	38.445	1.00	47.06	A
ATOM	2394	O	LEU	A	304	-31.258	16.420	39.126	1.00	47.06	A
ATOM	2395	N	ALA	A	305	-30.648	14.902	37.587	1.00	53.87	A
ATOM	2396	CA	ALA	A	305	-32.016	14.419	37.420	1.00	53.87	A
ATOM	2397	CB	ALA	A	305	-32.099	13.444	36.235	1.00	44.21	A
ATOM	2398	C	ALA	A	305	-32.502	13.736	38.697	1.00	53.87	A
ATOM	2399	O	ALA	A	305	-33.683	13.806	39.036	1.00	53.87	A
ATOM	2400	N	GLU	A	306	-31.579	13.092	39.408	1.00	52.70	A
ATOM	2401	CA	GLU	A	306	-31.895	12.382	40.643	1.00	52.70	A
ATOM	2402	CB	GLU	A	306	-30.826	11.311	40.889	1.00	68.37	A
ATOM	2403	CG	GLU	A	306	-31.346	10.015	41.479	1.00	68.37	A
ATOM	2404	CD	GLU	A	306	-32.508	9.440	40.692	1.00	68.37	A
ATOM	2405	OE1	GLU	A	306	-32.331	9.111	39.500	1.00	68.37	A
ATOM	2406	OE2	GLU	A	306	-33.607	9.322	41.272	1.00	68.37	A
ATOM	2407	C	GLU	A	306	-32.015	13.315	41.860	1.00	52.70	A
ATOM	2408	O	GLU	A	306	-32.555	12.923	42.894	1.00	52.70	A
ATOM	2409	N	VAL	A	307	-31.510	14.542	41.747	1.00	64.37	A
ATOM	2410	CA	VAL	A	307	-31.605	15.497	42.851	1.00	64.37	A
ATOM	2411	CB	VAL	A	307	-30.570	16.650	42.709	1.00	45.19	A
ATOM	2412	CG1	VAL	A	307	-30.814	17.716	43.769	1.00	45.19	A
ATOM	2413	CG2	VAL	A	307	-29.154	16.098	42.838	1.00	45.19	A
ATOM	2414	C	VAL	A	307	-33.018	16.078	42.827	1.00	64.37	A
ATOM	2415	O	VAL	A	307	-33.411	16.742	41.866	1.00	64.37	A
ATOM	2416	N	ASP	A	308	-33.784	15.818	43.881	1.00	78.01	A
ATOM	2417	CA	ASP	A	308	-35.158	16.300	43.950	1.00	78.01	A
ATOM	2418	CB	ASP	A	308	-36.032	15.258	44.660	1.00109.90		A
ATOM	2419	CG	ASP	A	308	-37.509	15.396	44.319	1.00109.90		A
ATOM	2420	OD1	ASP	A	308	-37.862	15.270	43.125	1.00109.90		A
ATOM	2421	OD2	ASP	A	308	-38.316	15.624	45.244	1.00109.90		A
ATOM	2422	C	ASP	A	308	-35.250	17.646	44.670	1.00	78.01	A
ATOM	2423	O	ASP	A	308	-35.921	17.768	45.693	1.00	78.01	A
ATOM	2424	N	SER	A	309	-34.572	18.654	44.132	1.00	96.37	A
ATOM	2425	CA	SER	A	309	-34.587	19.985	44.731	1.00	96.37	A
ATOM	2426	CB	SER	A	309	-33.392	20.162	45.677	1.00	66.94	A
ATOM	2427	OG	SER	A	309	-33.396	21.440	46.294	1.00	66.94	A
ATOM	2428	C	SER	A	309	-34.546	21.048	43.647	1.00	96.37	A
ATOM	2429	O	SER	A	309	-33.884	20.879	42.624	1.00	96.37	A
ATOM	2430	N	ASP	A	310	-35.263	22.141	43.878	1.00	63.63	A
ATOM	2431	CA	ASP	A	310	-35.311	23.239	42.926	1.00	63.63	A
ATOM	2432	CB	ASP	A	310	-36.724	23.821	42.862	1.00124.85		A
ATOM	2433	CG	ASP	A	310	-37.093	24.598	44.114	1.00124.85		A
ATOM	2434	OD1	ASP	A	310	-37.104	24.003	45.214	1.00124.85		A
ATOM	2435	OD2	ASP	A	310	-37.369	25.809	43.994	1.00124.85		A
ATOM	2436	C	ASP	A	310	-34.330	24.336	43.329	1.00	63.63	A
ATOM	2437	O	ASP	A	310	-34.211	25.351	42.639	1.00	63.63	A
ATOM	2438	N	ILE	A	311	-33.626	24.134	44.442	1.00	57.09	A
ATOM	2439	CA	ILE	A	311	-32.669	25.136	44.910	1.00	57.09	A
ATOM	2440	CB	ILE	A	311	-32.072	24.752	46.283	1.00	68.75	A

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ATOM   2441  CG2 ILE A 311     -31.014  23.689  46.120  1.00 68.75      A
ATOM   2442  CG1 ILE A 311     -31.458  25.984  46.942  1.00 68.75      A
ATOM   2443  CD1 ILE A 311     -32.468  27.049  47.300  1.00 68.75      A
ATOM   2444  C   ILE A 311     -31.538  25.364  43.895  1.00 57.09      A
ATOM   2445  O   ILE A 311     -30.880  26.401  43.930  1.00 57.09      A
ATOM   2446  N   ILE A 312     -31.313  24.394  43.005  1.00 49.83      A
ATOM   2447  CA  ILE A 312     -30.297  24.520  41.952  1.00 49.83      A
ATOM   2448  CB  ILE A 312     -29.091  23.543  42.129  1.00 44.05      A
ATOM   2449  CG2 ILE A 312     -28.345  23.855  43.406  1.00 44.05      A
ATOM   2450  CG1 ILE A 312     -29.581  22.095  42.077  1.00 44.05      A
ATOM   2451  CD1 ILE A 312     -28.482  21.053  42.188  1.00 44.05      A
ATOM   2452  C   ILE A 312     -30.921  24.194  40.598  1.00 49.83      A
ATOM   2453  O   ILE A 312     -31.837  23.376  40.512  1.00 49.83      A
ATOM   2454  N   ASP A 313     -30.409  24.820  39.544  1.00 61.26      A
ATOM   2455  CA  ASP A 313     -30.907  24.568  38.199  1.00 61.26      A
ATOM   2456  CB  ASP A 313     -30.147  25.420  37.183  1.00 81.89      A
ATOM   2457  CG  ASP A 313     -30.753  26.806  37.017  1.00 81.89      A
ATOM   2458  OD1 ASP A 313     -31.077  27.455  38.040  1.00 81.89      A
ATOM   2459  OD2 ASP A 313     -30.900  27.248  35.858  1.00 81.89      A

ATOM   2460  C   ASP A 313     -30.780  23.092  37.861  1.00 61.26      A
ATOM   2461  O   ASP A 313     -30.002  22.367  38.481  1.00 61.26      A
ATOM   2462  N   LYS A 314     -31.550  22.651  36.874  1.00 58.31      A
ATOM   2463  CA  LYS A 314     -31.555  21.246  36.471  1.00 58.31      A
ATOM   2464  CB  LYS A 314     -32.964  20.854  36.022  1.00132.79      A
ATOM   2465  CG  LYS A 314     -33.545  21.781  34.965  1.00132.79      A
ATOM   2466  CD  LYS A 314     -34.952  21.369  34.574  1.00132.79      A
ATOM   2467  CE  LYS A 314     -35.524  22.302  33.519  1.00132.79      A
ATOM   2468  NZ  LYS A 314     -36.920  21.938  33.142  1.00132.79      A
ATOM   2469  C   LYS A 314     -30.554  20.907  35.372  1.00 58.31      A
ATOM   2470  O   LYS A 314     -30.297  19.739  35.098  1.00 58.31      A
ATOM   2471  N   SER A 315     -29.987  21.924  34.738  1.00 53.32      A
ATOM   2472  CA  SER A 315     -29.016  21.666  33.683  1.00 53.32      A
ATOM   2473  CB  SER A 315     -29.587  22.101  32.326  1.00 53.18      A
ATOM   2474  OG  SER A 315     -29.930  23.473  32.331  1.00 53.18      A
ATOM   2475  C   SER A 315     -27.678  22.355  33.941  1.00 53.32      A
ATOM   2476  O   SER A 315     -27.599  23.342  34.680  1.00 53.32      A
ATOM   2477  N   LEU A 316     -26.628  21.811  33.335  1.00 49.89      A
ATOM   2478  CA  LEU A 316     -25.277  22.350  33.467  1.00 49.89      A
ATOM   2479  CB  LEU A 316     -24.273  21.346  32.912  1.00 43.63      A
ATOM   2480  CG  LEU A 316     -24.223  19.999  33.633  1.00 43.63      A
ATOM   2481  CD1 LEU A 316     -23.395  19.019  32.811  1.00 43.63      A
ATOM   2482  CD2 LEU A 316     -23.638  20.186  35.041  1.00 43.63      A
ATOM   2483  C   LEU A 316     -25.129  23.677  32.723  1.00 49.89      A
ATOM   2484  O   LEU A 316     -25.695  23.859  31.646  1.00 49.89      A
ATOM   2485  N   SER A 317     -24.364  24.605  33.291  1.00 42.87      A
ATOM   2486  CA  SER A 317     -24.166  25.903  32.653  1.00 42.87      A
ATOM   2487  CB  SER A 317     -23.535  26.893  33.628  1.00 46.89      A
ATOM   2488  OG  SER A 317     -24.364  27.089  34.747  1.00 46.89      A
ATOM   2489  C   SER A 317     -23.252  25.777  31.443  1.00 42.87      A
ATOM   2490  O   SER A 317     -22.449  24.850  31.342  1.00 42.87      A
ATOM   2491  N   GLU A 318     -23.387  26.717  30.523  1.00 52.92      A
ATOM   2492  CA  GLU A 318     -22.546  26.746  29.338  1.00 52.92      A
ATOM   2493  CB  GLU A 318     -23.396  26.786  28.073  1.00 65.32      A
ATOM   2494  CG  GLU A 318     -24.597  25.883  28.122  1.00 65.32      A
ATOM   2495  CD  GLU A 318     -25.230  25.690  26.764  1.00 65.32      A
ATOM   2496  OE1 GLU A 318     -25.483  26.699  26.076  1.00 65.32      A
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ATOM   2497  OE2 GLU A 318     -25.478  24.523  26.393  1.00 65.32      A
ATOM   2498  C   GLU A 318     -21.778  28.048  29.475  1.00 52.92      A
ATOM   2499  O   GLU A 318     -22.210  28.945  30.196  1.00 52.92      A
ATOM   2500  N   ILE A 319     -20.643  28.168  28.802  1.00 42.77      A
ATOM   2501  CA  ILE A 319     -19.886  29.411  28.899  1.00 42.77      A
ATOM   2502  CB  ILE A 319     -18.871  29.362  30.072  1.00 47.55      A
ATOM   2503  CG2 ILE A 319     -17.739  28.389  29.745  1.00 47.55      A
ATOM   2504  CG1 ILE A 319     -18.295  30.759  30.326  1.00 47.55      A
ATOM   2505  CD1 ILE A 319     -17.438  30.865  31.581  1.00 47.55      A
ATOM   2506  C   ILE A 319     -19.153  29.694  27.596  1.00 42.77      A
ATOM   2507  O   ILE A 319     -18.750  28.781  26.886  1.00 42.77      A
ATOM   2508  N   GLU A 320     -18.998  30.967  27.269  1.00 53.70      A
ATOM   2509  CA  GLU A 320     -18.304  31.329  26.048  1.00 53.70      A
ATOM   2510  CB  GLU A 320     -18.747  32.716  25.581  1.00 79.12      A
ATOM   2511  CG  GLU A 320     -18.238  33.095  24.201  1.00 79.12      A
ATOM   2512  CD  GLU A 320     -18.813  34.414  23.717  1.00 79.12      A
ATOM   2513  OE1 GLU A 320     -18.512  35.462  24.329  1.00 79.12      A
ATOM   2514  OE2 GLU A 320     -19.575  34.399  22.726  1.00 79.12      A
ATOM   2515  C   GLU A 320     -16.816  31.329  26.350  1.00 53.70      A
ATOM   2516  O   GLU A 320     -16.374  31.945  27.318  1.00 53.70      A
ATOM   2517  N   VAL A 321     -16.055  30.621  25.527  1.00 54.10      A
ATOM   2518  CA  VAL A 321     -14.620  30.536  25.711  1.00 54.10      A
ATOM   2519  CB  VAL A 321     -14.174  29.067  26.004  1.00 40.96      A
ATOM   2520  CG1 VAL A 321     -15.018  28.481  27.118  1.00 40.96      A
ATOM   2521  CG2 VAL A 321     -14.275  28.220  24.760  1.00 40.96      A
ATOM   2522  C   VAL A 321     -13.892  31.038  24.465  1.00 54.10      A
ATOM   2523  O   VAL A 321     -14.487  31.175  23.388  1.00 54.10      A
ATOM   2524  N   GLU A 322     -12.605  31.322  24.628  1.00 50.68      A
ATOM   2525  CA  GLU A 322     -11.763  31.786  23.536  1.00 50.68      A
ATOM   2526  CB  GLU A 322     -10.832  32.906  24.012  1.00101.57      A
ATOM   2527  CG  GLU A 322     -11.453  34.292  24.060  1.00101.57      A
ATOM   2528  CD  GLU A 322     -11.649  34.886  22.677  1.00101.57      A
ATOM   2529  OE1 GLU A 322     -10.662  34.953  21.913  1.00101.57      A
ATOM   2530  OE2 GLU A 322     -12.786  35.290  22.354  1.00101.57      A
ATOM   2531  C   GLU A 322     -10.925  30.606  23.085  1.00 50.68      A
ATOM   2532  O   GLU A 322     -10.310  29.932  23.911  1.00 50.68      A
ATOM   2533  N   LYS A 323     -10.911  30.337  21.785  1.00 59.49      A
ATOM   2534  CA  LYS A 323     -10.105  29.241  21.270  1.00 59.49      A
ATOM   2535  CB  LYS A 323     -10.617  28.785  19.901  1.00 85.31      A
ATOM   2536  CG  LYS A 323     -11.995  28.148  19.941  1.00 85.31      A
ATOM   2537  CD  LYS A 323     -12.426  27.616  18.574  1.00 85.31      A
ATOM   2538  CE  LYS A 323     -12.598  28.740  17.553  1.00 85.31      A
ATOM   2539  NZ  LYS A 323     -13.134  28.250  16.247  1.00 85.31      A
ATOM   2540  C   LYS A 323      -8.687  29.786  21.154  1.00 59.49      A
ATOM   2541  O   LYS A 323      -8.479  30.993  21.271  1.00 59.49      A
ATOM   2542  N   ILE A 324      -7.713  28.906  20.951  1.00 55.83      A
ATOM   2543  CA  ILE A 324      -6.326  29.339  20.823  1.00 55.83      A
ATOM   2544  CB  ILE A 324      -5.417  28.644  21.873  1.00 54.86      A
ATOM   2545  CG2 ILE A 324      -3.964  29.066  21.675  1.00 54.86      A
ATOM   2546  CG1 ILE A 324      -5.882  29.014  23.285  1.00 54.86      A
ATOM   2547  CD1 ILE A 324      -5.103  28.336  24.374  1.00 54.86      A
ATOM   2548  C   ILE A 324      -5.849  29.005  19.413  1.00 55.83      A
ATOM   2549  O   ILE A 324      -5.957  27.860  18.972  1.00 55.83      A
ATOM   2550  N   ALA A 325      -5.328  30.014  18.719  1.00 63.86      A
ATOM   2551  CA  ALA A 325      -4.853  29.873  17.340  1.00 63.86      A
ATOM   2552  CB  ALA A 325      -4.255  31.201  16.867  1.00 53.96      A
ATOM   2553  C   ALA A 325      -3.855  28.745  17.113  1.00 63.86      A
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FIGURE 25 CON'T
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ATOM   2554  O   ALA A 325     -2.978  28.499  17.942  1.00 63.86      A
ATOM   2555  N   GLN A 326     -3.992  28.061  15.981  1.00 68.30      A
ATOM   2556  CA  GLN A 326     -3.095  26.963  15.639  1.00 68.30      A
ATOM   2557  CB  GLN A 326     -3.548  26.275  14.350  1.00137.18      A
ATOM   2558  CG  GLN A 326     -4.919  25.633  14.421  1.00137.18      A
ATOM   2559  CD  GLN A 326     -5.318  24.982  13.109  1.00137.18      A
ATOM   2560  OE1 GLN A 326     -5.411  25.645  12.076  1.00137.18      A
ATOM   2561  NE2 GLN A 326     -5.555  23.675  13.146  1.00137.18      A
ATOM   2562  C   GLN A 326     -1.691  27.513  15.444  1.00 68.30      A
ATOM   2563  O   GLN A 326     -0.710  26.777  15.522  1.00 68.30      A
ATOM   2564  N   GLU A 327     -1.608  28.817  15.193  1.00 63.72      A
ATOM   2565  CA  GLU A 327     -0.332  29.486  14.977  1.00 63.72      A
ATOM   2566  CB  GLU A 327     -0.561  30.941  14.564  1.00133.49      A
ATOM   2567  CG  GLU A 327      0.723  31.714  14.303  1.00133.49      A
ATOM   2568  CD  GLU A 327      0.503  33.215  14.263  1.00133.49      A
ATOM   2569  OE1 GLU A 327      1.459  33.950  13.933  1.00133.49      A
ATOM   2570  OE2 GLU A 327     -0.624  33.660  14.570  1.00133.49      A
ATOM   2571  C   GLU A 327      0.547  29.461  16.223  1.00 63.72      A
ATOM   2572  O   GLU A 327      1.763  29.316  16.126  1.00 63.72      A
ATOM   2573  N   LEU A 328     -0.074  29.623  17.389  1.00 61.48      A
ATOM   2574  CA  LEU A 328      0.660  29.628  18.653  1.00 61.48      A
ATOM   2575  CB  LEU A 328     -0.253  30.110  19.783  1.00 64.24      A
ATOM   2576  CG  LEU A 328     -0.757  31.547  19.614  1.00 64.24      A
ATOM   2577  CD1 LEU A 328     -1.830  31.866  20.646  1.00 64.24      A
ATOM   2578  CD2 LEU A 328      0.414  32.506  19.744  1.00 64.24      A
ATOM   2579  C   LEU A 328      1.218  28.241  18.972  1.00 61.48      A
ATOM   2580  O   LEU A 328      1.834  28.032  20.010  1.00 61.48      A
ATOM   2581  N   GLU A 329      1.001  27.307  18.053  1.00 61.19      A
ATOM   2582  CA  GLU A 329      1.464  25.935  18.187  1.00 61.19      A
ATOM   2583  CB  GLU A 329      0.471  24.975  17.529  1.00 79.60      A
ATOM   2584  CG  GLU A 329     -0.875  24.863  18.200  1.00 79.60      A
ATOM   2585  CD  GLU A 329     -0.838  23.942  19.394  1.00 79.60      A
ATOM   2586  OE1 GLU A 329     -0.423  22.776  19.229  1.00 79.60      A
ATOM   2587  OE2 GLU A 329     -1.224  24.382  20.494  1.00 79.60      A

ATOM   2588  C   GLU A 329      2.793  25.773  17.470  1.00 61.19      A
ATOM   2589  O   GLU A 329      3.492  24.778  17.667  1.00 61.19      A
ATOM   2590  N   ASN A 330      3.143  26.749  16.638  1.00 55.96      A
ATOM   2591  CA  ASN A 330      4.369  26.640  15.858  1.00 55.96      A
ATOM   2592  CB  ASN A 330      4.044  26.811  14.366  1.00 70.78      A
ATOM   2593  CG  ASN A 330      2.756  26.108  13.956  1.00 70.78      A
ATOM   2594  OD1 ASN A 330      2.566  24.921  14.218  1.00 70.78      A
ATOM   2595  ND2 ASN A 330      1.864  26.848  13.304  1.00 70.78      A
ATOM   2596  C   ASN A 330      5.488  27.605  16.232  1.00 55.96      A
ATOM   2597  O   ASN A 330      6.381  27.849  15.425  1.00 55.96      A
ATOM   2598  N   LYS A 331      5.462  28.143  17.443  1.00 43.12      A
ATOM   2599  CA  LYS A 331      6.495  29.095  17.831  1.00 43.12      A
ATOM   2600  CB  LYS A 331      5.958  30.016  18.924  1.00 70.20      A
ATOM   2601  CG  LYS A 331      4.812  30.887  18.417  1.00 70.20      A
ATOM   2602  CD  LYS A 331      4.619  32.131  19.261  1.00 70.20      A
ATOM   2603  CE  LYS A 331      3.665  33.108  18.578  1.00 70.20      A
ATOM   2604  NZ  LYS A 331      4.143  33.510  17.219  1.00 70.20      A
ATOM   2605  C   LYS A 331      7.840  28.490  18.237  1.00 43.12      A
ATOM   2606  O   LYS A 331      8.846  29.201  18.325  1.00 43.12      A
ATOM   2607  N   ILE A 332      7.870  27.176  18.449  1.00 45.53      A
ATOM   2608  CA  ILE A 332      9.100  26.502  18.836  1.00 45.53      A
ATOM   2609  CB  ILE A 332      8.854  25.576  20.054  1.00 52.84      A
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FIGURE 25 CON'T

ATOM	2610	CG2	ILE	A	332	10.114	24.772	20.382	1.00	52.84	A
ATOM	2611	CG1	ILE	A	332	8.417	26.419	21.254	1.00	52.84	A
ATOM	2612	CD1	ILE	A	332	7.900	25.599	22.417	1.00	52.84	A
ATOM	2613	C	ILE	A	332	9.609	25.676	17.666	1.00	45.53	A
ATOM	2614	O	ILE	A	332	8.909	24.787	17.184	1.00	45.53	A
ATOM	2615	N	ARG	A	333	10.829	25.956	17.214	1.00	45.17	A
ATOM	2616	CA	ARG	A	333	11.383	25.215	16.082	1.00	45.17	A
ATOM	2617	CB	ARG	A	333	11.418	26.112	14.837	1.00	93.38	A
ATOM	2618	CG	ARG	A	333	10.064	26.641	14.388	1.00	93.38	A
ATOM	2619	CD	ARG	A	333	10.141	27.407	13.060	1.00	93.38	A
ATOM	2620	NE	ARG	A	333	10.929	28.637	13.145	1.00	93.38	A
ATOM	2621	CZ	ARG	A	333	12.258	28.691	13.082	1.00	93.38	A
ATOM	2622	NH1	ARG	A	333	12.967	27.581	12.928	1.00	93.38	A
ATOM	2623	NH2	ARG	A	333	12.882	29.859	13.178	1.00	93.38	A
ATOM	2624	C	ARG	A	333	12.781	24.624	16.291	1.00	45.17	A
ATOM	2625	O	ARG	A	333	13.519	25.027	17.202	1.00	45.17	A
ATOM	2626	N	VAL	A	334	13.123	23.664	15.429	1.00	59.14	A
ATOM	2627	CA	VAL	A	334	14.430	23.013	15.430	1.00	59.14	A
ATOM	2628	CB	VAL	A	334	14.369	21.557	15.970	1.00	47.97	A
ATOM	2629	CG1	VAL	A	334	14.003	21.570	17.456	1.00	47.97	A
ATOM	2630	CG2	VAL	A	334	13.363	20.736	15.173	1.00	47.97	A
ATOM	2631	C	VAL	A	334	14.925	23.001	13.986	1.00	59.14	A
ATOM	2632	O	VAL	A	334	14.134	23.150	13.051	1.00	59.14	A
ATOM	2633	N	ARG	A	335	16.225	22.816	13.794	1.00	54.77	A
ATOM	2634	CA	ARG	A	335	16.785	22.827	12.451	1.00	54.77	A
ATOM	2635	CB	ARG	A	335	17.499	24.162	12.214	1.00	63.65	A
ATOM	2636	CG	ARG	A	335	18.598	24.412	13.240	1.00	63.65	A
ATOM	2637	CD	ARG	A	335	19.398	25.676	12.990	1.00	63.65	A
ATOM	2638	NE	ARG	A	335	20.376	25.881	14.056	1.00	63.65	A
ATOM	2639	CZ	ARG	A	335	21.342	26.795	14.035	1.00	63.65	A
ATOM	2640	NH1	ARG	A	335	21.475	27.605	12.997	1.00	63.65	A
ATOM	2641	NH2	ARG	A	335	22.185	26.893	15.053	1.00	63.65	A
ATOM	2642	C	ARG	A	335	17.777	21.690	12.237	1.00	54.77	A
ATOM	2643	O	ARG	A	335	18.200	21.041	13.196	1.00	54.77	A
ATOM	2644	N	ASP	A	336	18.145	21.464	10.973	1.00	57.09	A
ATOM	2645	CA	ASP	A	336	19.117	20.430	10.615	1.00	57.09	A
ATOM	2646	CB	ASP	A	336	18.614	19.589	9.438	1.00	89.22	A
ATOM	2647	CG	ASP	A	336	18.159	20.434	8.268	1.00	89.22	A
ATOM	2648	OD1	ASP	A	336	18.929	21.312	7.826	1.00	89.22	A
ATOM	2649	OD2	ASP	A	336	17.029	20.211	7.787	1.00	89.22	A
ATOM	2650	C	ASP	A	336	20.451	21.098	10.258	1.00	57.09	A
ATOM	2651	O	ASP	A	336	20.592	22.317	10.399	1.00	57.09	A
ATOM	2652	N	ASP	A	337	21.425	20.309	9.807	1.00	74.53	A
ATOM	2653	CA	ASP	A	337	22.740	20.852	9.461	1.00	74.53	A
ATOM	2654	CB	ASP	A	337	23.794	19.739	9.446	1.00	86.24	A
ATOM	2655	CG	ASP	A	337	23.462	18.634	8.468	1.00	86.24	A
ATOM	2656	OD1	ASP	A	337	22.338	18.093	8.540	1.00	86.24	A
ATOM	2657	OD2	ASP	A	337	24.327	18.301	7.629	1.00	86.24	A
ATOM	2658	C	ASP	A	337	22.741	21.590	8.127	1.00	74.53	A
ATOM	2659	O	ASP	A	337	23.748	22.183	7.739	1.00	74.53	A
ATOM	2660	N	LYS	A	338	21.613	21.542	7.426	1.00	94.53	A
ATOM	2661	CA	LYS	A	338	21.476	22.235	6.152	1.00	94.53	A
ATOM	2662	CB	LYS	A	338	20.460	21.527	5.249	1.00	92.71	A
ATOM	2663	CG	LYS	A	338	20.999	20.319	4.490	1.00	92.71	A
ATOM	2664	CD	LYS	A	338	21.334	19.151	5.402	1.00	92.71	A
ATOM	2665	CE	LYS	A	338	21.821	17.954	4.592	1.00	92.71	A
ATOM	2666	NZ	LYS	A	338	22.167	16.779	5.444	1.00	92.71	A

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ATOM	2667	C	LYS	A	338	20.997	23.648	6.452	1.00	94.53	A
ATOM	2668	O	LYS	A	338	21.757	24.481	6.944	1.00	94.53	A
ATOM	2669	N	GLY	A	339	19.728	23.908	6.165	1.00	93.63	A
ATOM	2670	CA	GLY	A	339	19.164	25.219	6.423	1.00	93.63	A
ATOM	2671	C	GLY	A	339	17.670	25.120	6.645	1.00	93.63	A
ATOM	2672	O	GLY	A	339	16.958	26.123	6.594	1.00	93.63	A
ATOM	2673	N	ASN	A	340	17.196	23.904	6.902	1.00	66.46	A
ATOM	2674	CA	ASN	A	340	15.773	23.665	7.122	1.00	66.46	A
ATOM	2675	CB	ASN	A	340	15.409	22.247	6.684	1.00	93.09	A
ATOM	2676	CG	ASN	A	340	15.896	21.929	5.290	1.00	93.09	A
ATOM	2677	OD1	ASN	A	340	17.097	21.962	5.019	1.00	93.09	A
ATOM	2678	ND2	ASN	A	340	14.968	21.618	4.393	1.00	93.09	A
ATOM	2679	C	ASN	A	340	15.326	23.878	8.570	1.00	66.46	A
ATOM	2680	O	ASN	A	340	15.940	23.366	9.510	1.00	66.46	A
ATOM	2681	N	SER	A	341	14.245	24.635	8.729	1.00	90.87	A
ATOM	2682	CA	SER	A	341	13.675	24.928	10.036	1.00	90.87	A
ATOM	2683	CB	SER	A	341	13.751	26.424	10.334	1.00	97.06	A
ATOM	2684	OG	SER	A	341	15.093	26.865	10.405	1.00	97.06	A
ATOM	2685	C	SER	A	341	12.218	24.493	10.047	1.00	90.87	A
ATOM	2686	O	SER	A	341	11.420	24.942	9.226	1.00	90.87	A
ATOM	2687	N	VAL	A	342	11.878	23.613	10.978	1.00	73.22	A
ATOM	2688	CA	VAL	A	342	10.516	23.120	11.106	1.00	73.22	A
ATOM	2689	CB	VAL	A	342	10.406	21.658	10.608	1.00	84.47	A
ATOM	2690	CG1	VAL	A	342	9.030	21.096	10.927	1.00	84.47	A
ATOM	2691	CG2	VAL	A	342	10.665	21.602	9.107	1.00	84.47	A
ATOM	2692	C	VAL	A	342	10.096	23.185	12.570	1.00	73.22	A
ATOM	2693	O	VAL	A	342	10.889	22.889	13.461	1.00	73.22	A
ATOM	2694	N	PRO	A	343	8.847	23.599	12.837	1.00	65.78	A
ATOM	2695	CD	PRO	A	343	7.871	24.164	11.886	1.00	66.06	A
ATOM	2696	CA	PRO	A	343	8.350	23.689	14.215	1.00	65.78	A
ATOM	2697	CB	PRO	A	343	7.115	24.574	14.075	1.00	66.06	A
ATOM	2698	CG	PRO	A	343	6.605	24.214	12.708	1.00	66.06	A
ATOM	2699	C	PRO	A	343	8.017	22.302	14.771	1.00	65.78	A
ATOM	2700	O	PRO	A	343	7.633	21.401	14.019	1.00	65.78	A
ATOM	2701	N	ILE	A	344	8.176	22.130	16.083	1.00	66.21	A
ATOM	2702	CA	ILE	A	344	7.889	20.849	16.718	1.00	66.21	A
ATOM	2703	CB	ILE	A	344	8.027	20.936	18.268	1.00	95.56	A
ATOM	2704	CG2	ILE	A	344	7.364	19.732	18.928	1.00	95.56	A
ATOM	2705	CG1	ILE	A	344	9.503	20.977	18.670	1.00	95.56	A
ATOM	2706	CD1	ILE	A	344	10.266	22.154	18.127	1.00	95.56	A
ATOM	2707	C	ILE	A	344	6.473	20.411	16.361	1.00	66.21	A
ATOM	2708	O	ILE	A	344	5.504	20.847	16.984	1.00	66.21	A
ATOM	2709	N	SER	A	345	6.367	19.555	15.347	1.00	132.27	A
ATOM	2710	CA	SER	A	345	5.085	19.033	14.877	1.00	132.27	A
ATOM	2711	CB	SER	A	345	4.191	20.171	14.377	1.00	71.12	A
ATOM	2712	OG	SER	A	345	3.918	21.114	15.400	1.00	71.12	A
ATOM	2713	C	SER	A	345	5.304	18.036	13.739	1.00	132.27	A
ATOM	2714	O	SER	A	345	5.223	18.400	12.566	1.00	132.27	A
ATOM	2715	N	GLN	A	346	5.587	16.783	14.087	1.00	139.05	A
ATOM	2716	CA	GLN	A	346	5.811	15.745	13.085	1.00	139.05	A
ATOM	2717	CB	GLN	A	346	7.228	15.171	13.204	1.00	115.07	A
ATOM	2718	CG	GLN	A	346	8.344	16.209	13.198	1.00	115.07	A
ATOM	2719	CD	GLN	A	346	8.739	16.660	14.595	1.00	115.07	A
ATOM	2720	OE1	GLN	A	346	7.906	17.122	15.372	1.00	115.07	A
ATOM	2721	NE2	GLN	A	346	10.020	16.527	14.918	1.00	115.07	A
ATOM	2722	C	GLN	A	346	4.794	14.616	13.241	1.00	139.05	A

ATOM	2723	O	GLN	A	346	5.005	13.504	12.757	1.00	139.05	A
ATOM	2724	N	LEU	A	355	9.591	8.875	-2.331	1.00	72.02	A
ATOM	2725	CA	LEU	A	355	10.136	9.754	-1.302	1.00	72.02	A
ATOM	2726	CB	LEU	A	355	9.665	9.304	0.089	1.00	78.63	A
ATOM	2727	CG	LEU	A	355	8.508	10.101	0.702	1.00	78.63	A
ATOM	2728	CD1	LEU	A	355	7.944	9.358	1.900	1.00	78.63	A
ATOM	2729	CD2	LEU	A	355	9.000	11.491	1.112	1.00	78.63	A
ATOM	2730	C	LEU	A	355	11.663	9.823	-1.343	1.00	72.02	A
ATOM	2731	O	LEU	A	355	12.309	9.182	-2.179	1.00	72.02	A
ATOM	2732	N	LEU	A	356	12.225	10.611	-0.430	1.00	65.93	A
ATOM	2733	CA	LEU	A	356	13.667	10.810	-0.330	1.00	65.93	A
ATOM	2734	CB	LEU	A	356	13.992	11.618	0.931	1.00	79.78	A
ATOM	2735	CG	LEU	A	356	15.435	12.095	1.087	1.00	79.78	A
ATOM	2736	CD1	LEU	A	356	15.775	13.058	-0.039	1.00	79.78	A
ATOM	2737	CD2	LEU	A	356	15.609	12.772	2.437	1.00	79.78	A
ATOM	2738	C	LEU	A	356	14.447	9.496	-0.318	1.00	65.93	A
ATOM	2739	O	LEU	A	356	14.209	8.617	0.514	1.00	65.93	A
ATOM	2740	N	TRP	A	357	15.394	9.387	-1.245	1.00	61.77	A
ATOM	2741	CA	TRP	A	357	16.223	8.199	-1.391	1.00	61.77	A
ATOM	2742	CB	TRP	A	357	17.331	8.470	-2.422	1.00	64.38	A
ATOM	2743	CG	TRP	A	357	18.220	9.633	-2.077	1.00	64.38	A
ATOM	2744	CD2	TRP	A	357	19.646	9.611	-1.936	1.00	64.38	A
ATOM	2745	CE2	TRP	A	357	20.055	10.924	-1.611	1.00	64.38	A
ATOM	2746	CE3	TRP	A	357	20.619	8.610	-2.053	1.00	64.38	A
ATOM	2747	CD1	TRP	A	357	17.833	10.926	-1.838	1.00	64.38	A
ATOM	2748	NE1	TRP	A	357	18.930	11.705	-1.558	1.00	64.38	A
ATOM	2749	CZ2	TRP	A	357	21.396	11.262	-1.401	1.00	64.38	A
ATOM	2750	CZ3	TRP	A	357	21.952	8.946	-1.845	1.00	64.38	A
ATOM	2751	CH2	TRP	A	357	22.327	10.264	-1.522	1.00	64.38	A
ATOM	2752	C	TRP	A	357	16.842	7.679	-0.089	1.00	61.77	A
ATOM	2753	O	TRP	A	357	16.840	6.468	0.161	1.00	61.77	A
ATOM	2754	N	THR	A	358	17.356	8.590	0.738	1.00	70.70	A
ATOM	2755	CA	THR	A	358	18.007	8.224	2.000	1.00	70.70	A
ATOM	2756	CB	THR	A	358	18.856	9.400	2.550	1.00	65.54	A
ATOM	2757	OG1	THR	A	358	18.031	10.564	2.680	1.00	65.54	A
ATOM	2758	CG2	THR	A	358	20.027	9.705	1.617	1.00	65.54	A
ATOM	2759	C	THR	A	358	17.094	7.746	3.132	1.00	70.70	A
ATOM	2760	O	THR	A	358	17.583	7.380	4.204	1.00	70.70	A
ATOM	2761	N	ASN	A	359	15.782	7.737	2.901	1.00	67.73	A
ATOM	2762	CA	ASN	A	359	14.826	7.311	3.929	1.00	67.73	A
ATOM	2763	CB	ASN	A	359	13.395	7.636	3.497	1.00	74.30	A
ATOM	2764	CG	ASN	A	359	13.145	9.127	3.384	1.00	74.30	A
ATOM	2765	OD1	ASN	A	359	13.878	9.935	3.956	1.00	74.30	A
ATOM	2766	ND2	ASN	A	359	12.107	9.498	2.643	1.00	78.38	A
ATOM	2767	C	ASN	A	359	14.862	5.820	4.260	1.00	67.73	A
ATOM	2768	O	ASN	A	359	14.010	5.323	4.993	1.00	67.73	A
ATOM	2769	N	TYR	A	360	15.847	5.105	3.730	1.00	69.19	A
ATOM	2770	CA	TYR	A	360	15.956	3.673	3.988	1.00	69.19	A
ATOM	2771	CB	TYR	A	360	16.561	2.970	2.774	1.00	54.50	A
ATOM	2772	CG	TYR	A	360	18.044	3.230	2.629	1.00	54.50	A
ATOM	2773	CD1	TYR	A	360	18.984	2.349	3.168	1.00	54.50	A
ATOM	2774	CE1	TYR	A	360	20.352	2.617	3.085	1.00	54.50	A
ATOM	2775	CD2	TYR	A	360	18.508	4.385	2.003	1.00	54.50	A
ATOM	2776	CE2	TYR	A	360	19.871	4.662	1.917	1.00	54.50	A
ATOM	2777	CZ	TYR	A	360	20.785	3.774	2.458	1.00	54.50	A
ATOM	2778	OH	TYR	A	360	22.129	4.041	2.356	1.00	54.50	A
ATOM	2779	C	TYR	A	360	16.832	3.379	5.203	1.00	69.19	A

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ATOM	2780	O	TYR	A	360	16.650	2.362	5.868	1.00	69.19	A
ATOM	2781	N	SER	A	361	17.782	4.268	5.486	1.00	60.27	A
ATOM	2782	CA	SER	A	361	18.713	4.061	6.597	1.00	60.27	A
ATOM	2783	CB	SER	A	361	19.987	4.898	6.387	1.00	72.15	A
ATOM	2784	OG	SER	A	361	19.745	6.275	6.608	1.00	72.15	A
ATOM	2785	C	SER	A	361	18.165	4.328	8.001	1.00	60.27	A
ATOM	2786	O	SER	A	361	17.225	5.104	8.191	1.00	60.27	A
ATOM	2787	N	ARG	A	362	18.786	3.671	8.979	1.00	65.79	A
ATOM	2788	CA	ARG	A	362	18.413	3.798	10.386	1.00	65.79	A
ATOM	2789	CB	ARG	A	362	18.830	2.537	11.153	1.00	83.77	A
ATOM	2790	CG	ARG	A	362	17.866	1.358	11.048	1.00	83.77	A
ATOM	2791	CD	ARG	A	362	17.631	0.927	9.612	1.00	83.77	A
ATOM	2792	NE	ARG	A	362	16.788	-0.264	9.522	1.00	83.77	A
ATOM	2793	CZ	ARG	A	362	17.185	-1.497	9.825	1.00	83.77	A
ATOM	2794	NH1	ARG	A	362	18.423	-1.718	10.244	1.00	83.77	A
ATOM	2795	NH2	ARG	A	362	16.343	-2.514	9.699	1.00	83.77	A
ATOM	2796	C	ARG	A	362	19.060	5.022	11.034	1.00	65.79	A
ATOM	2797	O	ARG	A	362	19.064	5.154	12.255	1.00	65.79	A
ATOM	2798	N	LYS	A	363	19.610	5.914	10.216	1.00	54.37	A
ATOM	2799	CA	LYS	A	363	20.257	7.123	10.723	1.00	54.37	A
ATOM	2800	CB	LYS	A	363	20.897	7.902	9.568	1.00	103.89	A
ATOM	2801	CG	LYS	A	363	21.841	7.073	8.710	1.00	103.89	A
ATOM	2802	CD	LYS	A	363	22.262	7.820	7.448	1.00	103.89	A
ATOM	2803	CE	LYS	A	363	23.043	6.914	6.492	1.00	103.89	A
ATOM	2804	NZ	LYS	A	363	23.344	7.575	5.185	1.00	103.89	A
ATOM	2805	C	LYS	A	363	19.225	8.004	11.421	1.00	54.37	A
ATOM	2806	O	LYS	A	363	18.150	8.256	10.877	1.00	54.37	A
ATOM	2807	N	TYR	A	364	19.543	8.464	12.627	1.00	54.01	A
ATOM	2808	CA	TYR	A	364	18.627	9.331	13.363	1.00	54.01	A
ATOM	2809	CB	TYR	A	364	19.116	9.539	14.802	1.00	44.05	A
ATOM	2810	CG	TYR	A	364	18.352	8.759	15.845	1.00	44.05	A
ATOM	2811	CD1	TYR	A	364	17.691	9.416	16.888	1.00	44.05	A
ATOM	2812	CE1	TYR	A	364	16.968	8.710	17.838	1.00	44.05	A
ATOM	2813	CD2	TYR	A	364	18.272	7.373	15.784	1.00	44.05	A
ATOM	2814	CE2	TYR	A	364	17.551	6.659	16.732	1.00	44.05	A
ATOM	2815	CZ	TYR	A	364	16.899	7.334	17.755	1.00	44.05	A
ATOM	2816	OH	TYR	A	364	16.160	6.623	18.677	1.00	44.05	A
ATOM	2817	C	TYR	A	364	18.572	10.683	12.669	1.00	54.01	A
ATOM	2818	O	TYR	A	364	19.467	11.025	11.899	1.00	54.01	A
ATOM	2819	N	PRO	A	365	17.509	11.466	12.915	1.00	54.14	A
ATOM	2820	CD	PRO	A	365	16.304	11.223	13.730	1.00	56.06	A
ATOM	2821	CA	PRO	A	365	17.451	12.775	12.262	1.00	54.14	A
ATOM	2822	CB	PRO	A	365	16.075	13.309	12.666	1.00	56.06	A
ATOM	2823	CG	PRO	A	365	15.815	12.628	14.004	1.00	56.06	A
ATOM	2824	C	PRO	A	365	18.589	13.631	12.808	1.00	54.14	A
ATOM	2825	O	PRO	A	365	19.115	13.355	13.887	1.00	54.14	A
ATOM	2826	N	VAL	A	366	18.977	14.656	12.058	1.00	60.13	A
ATOM	2827	CA	VAL	A	366	20.048	15.537	12.487	1.00	60.13	A
ATOM	2828	CB	VAL	A	366	20.995	15.884	11.321	1.00	76.49	A
ATOM	2829	CG1	VAL	A	366	22.142	16.744	11.824	1.00	76.49	A
ATOM	2830	CG2	VAL	A	366	21.521	14.608	10.682	1.00	76.49	A
ATOM	2831	C	VAL	A	366	19.456	16.825	13.036	1.00	60.13	A
ATOM	2832	O	VAL	A	366	18.631	17.471	12.389	1.00	60.13	A
ATOM	2833	N	ILE	A	367	19.887	17.188	14.237	1.00	56.80	A
ATOM	2834	CA	ILE	A	367	19.416	18.392	14.892	1.00	56.80	A
ATOM	2835	CB	ILE	A	367	18.727	18.042	16.233	1.00	56.93	A
ATOM	2836	CG2	ILE	A	367	18.512	19.289	17.077	1.00	56.93	A

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ATOM	2837	CG1	ILE	A	367	17.397	17.341	15.952	1.00	56.93	A
ATOM	2838	CD1	ILE	A	367	16.394	18.190	15.180	1.00	56.93	A
ATOM	2839	C	ILE	A	367	20.614	19.294	15.133	1.00	56.80	A
ATOM	2840	O	ILE	A	367	21.596	18.885	15.745	1.00	56.80	A
ATOM	2841	N	LEU	A	368	20.537	20.523	14.642	1.00	55.93	A
ATOM	2842	CA	LEU	A	368	21.632	21.467	14.814	1.00	55.93	A
ATOM	2843	CB	LEU	A	368	21.925	22.170	13.484	1.00	64.80	A
ATOM	2844	CG	LEU	A	368	23.235	22.948	13.340	1.00	64.80	A
ATOM	2845	CD1	LEU	A	368	23.180	24.216	14.165	1.00	64.80	A
ATOM	2846	CD2	LEU	A	368	24.404	22.066	13.767	1.00	64.80	A
ATOM	2847	C	LEU	A	368	21.249	22.479	15.886	1.00	55.93	A
ATOM	2848	O	LEU	A	368	20.405	23.349	15.664	1.00	55.93	A
ATOM	2849	N	PRO	A	369	21.871	22.375	17.070	1.00	54.36	A
ATOM	2850	CD	PRO	A	369	22.843	21.326	17.416	1.00	55.34	A
ATOM	2851	CA	PRO	A	369	21.630	23.254	18.221	1.00	54.36	A
ATOM	2852	CB	PRO	A	369	22.542	22.668	19.302	1.00	55.34	A
ATOM	2853	CG	PRO	A	369	22.670	21.230	18.906	1.00	55.34	A
ATOM	2854	C	PRO	A	369	21.928	24.738	17.978	1.00	54.36	A
ATOM	2855	O	PRO	A	369	22.768	25.099	17.148	1.00	54.36	A
ATOM	2856	N	TYR	A	370	21.235	25.593	18.717	1.00	56.23	A
ATOM	2857	CA	TYR	A	370	21.439	27.027	18.606	1.00	56.23	A
ATOM	2858	CB	TYR	A	370	20.132	27.767	18.899	1.00	65.92	A
ATOM	2859	CG	TYR	A	370	19.095	27.540	17.824	1.00	65.92	A
ATOM	2860	CD1	TYR	A	370	19.116	28.281	16.638	1.00	65.92	A
ATOM	2861	CE1	TYR	A	370	18.216	28.016	15.607	1.00	65.92	A
ATOM	2862	CD2	TYR	A	370	18.143	26.530	17.952	1.00	65.92	A
ATOM	2863	CE2	TYR	A	370	17.244	26.254	16.929	1.00	65.92	A
ATOM	2864	CZ	TYR	A	370	17.286	26.999	15.758	1.00	65.92	A
ATOM	2865	OH	TYR	A	370	16.409	26.712	14.741	1.00	65.92	A
ATOM	2866	C	TYR	A	370	22.514	27.408	19.612	1.00	56.23	A
ATOM	2867	O	TYR	A	370	23.215	28.404	19.439	1.00	56.23	A
ATOM	2868	N	GLU	A	371	22.633	26.594	20.661	1.00	62.81	A
ATOM	2869	CA	GLU	A	371	23.626	26.800	21.713	1.00	62.81	A
ATOM	2870	CB	GLU	A	371	23.072	27.693	22.829	1.00	68.13	A
ATOM	2871	CG	GLU	A	371	22.935	29.166	22.486	1.00	68.13	A
ATOM	2872	CD	GLU	A	371	22.631	30.018	23.714	1.00	68.13	A
ATOM	2873	OE1	GLU	A	371	23.351	29.875	24.724	1.00	68.13	A
ATOM	2874	OE2	GLU	A	371	21.683	30.830	23.673	1.00	68.13	A
ATOM	2875	C	GLU	A	371	24.045	25.466	22.325	1.00	62.81	A
ATOM	2876	O	GLU	A	371	23.224	24.562	22.500	1.00	62.81	A
ATOM	2877	N	VAL	A	372	25.329	25.351	22.647	1.00	53.69	A
ATOM	2878	CA	VAL	A	372	25.868	24.145	23.262	1.00	53.69	A
ATOM	2879	CB	VAL	A	372	26.710	23.327	22.262	1.00	45.98	A
ATOM	2880	CG1	VAL	A	372	27.399	22.165	22.975	1.00	45.98	A
ATOM	2881	CG2	VAL	A	372	25.823	22.800	21.152	1.00	45.98	A
ATOM	2882	C	VAL	A	372	26.757	24.580	24.419	1.00	53.69	A
ATOM	2883	O	VAL	A	372	27.671	25.385	24.232	1.00	53.69	A
ATOM	2884	N	PRO	A	373	26.492	24.067	25.636	1.00	56.69	A
ATOM	2885	CD	PRO	A	373	25.482	23.052	25.996	1.00	56.28	A
ATOM	2886	CA	PRO	A	373	27.304	24.431	26.803	1.00	56.69	A
ATOM	2887	CB	PRO	A	373	26.997	23.308	27.789	1.00	56.28	A
ATOM	2888	CG	PRO	A	373	25.545	23.047	27.516	1.00	56.28	A
ATOM	2889	C	PRO	A	373	28.783	24.491	26.419	1.00	56.69	A
ATOM	2890	O	PRO	A	373	29.285	23.612	25.716	1.00	56.69	A
ATOM	2891	N	GLU	A	374	29.474	25.534	26.861	1.00	69.16	A
ATOM	2892	CA	GLU	A	374	30.883	25.675	26.525	1.00	69.16	A

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ATOM	2893	CB	GLU	A	374	31.386	27.050	26.977	1.00135.63	A
ATOM	2894	CG	GLU	A	374	30.655	28.197	26.279	1.00135.63	A
ATOM	2895	CD	GLU	A	374	31.132	29.570	26.712	1.00135.63	A
ATOM	2896	OE1	GLU	A	374	31.019	29.893	27.913	1.00135.63	A
ATOM	2897	OE2	GLU	A	374	31.616	30.331	25.848	1.00135.63	A
ATOM	2898	C	GLU	A	374	31.706	24.545	27.143	1.00 69.16	A
ATOM	2899	O	GLU	A	374	32.843	24.295	26.743	1.00 69.16	A
ATOM	2900	N	LYS	A	375	31.105	23.847	28.102	1.00 88.08	A
ATOM	2901	CA	LYS	A	375	31.758	22.734	28.777	1.00 88.08	A
ATOM	2902	CB	LYS	A	375	30.815	22.126	29.814	1.00112.71	A
ATOM	2903	CG	LYS	A	375	31.323	20.817	30.386	1.00112.71	A
ATOM	2904	CD	LYS	A	375	30.267	20.112	31.208	1.00112.71	A
ATOM	2905	CE	LYS	A	375	30.738	18.723	31.593	1.00112.71	A
ATOM	2906	NZ	LYS	A	375	31.981	18.761	32.414	1.00112.71	A
ATOM	2907	C	LYS	A	375	32.205	21.638	27.813	1.00 88.08	A
ATOM	2908	O	LYS	A	375	33.281	21.061	27.974	1.00 88.08	A
ATOM	2909	N	PHE	A	376	31.373	21.349	26.817	1.00 74.38	A
ATOM	2910	CA	PHE	A	376	31.669	20.305	25.840	1.00 74.38	A
ATOM	2911	CB	PHE	A	376	30.433	20.041	24.972	1.00 57.91	A
ATOM	2912	CG	PHE	A	376	29.296	19.419	25.719	1.00 57.91	A
ATOM	2913	CD1	PHE	A	376	29.330	18.076	26.065	1.00 57.91	A
ATOM	2914	CD2	PHE	A	376	28.210	20.184	26.119	1.00 57.91	A
ATOM	2915	CE1	PHE	A	376	28.297	17.503	26.803	1.00 57.91	A
ATOM	2916	CE2	PHE	A	376	27.172	19.621	26.858	1.00 57.91	A
ATOM	2917	CZ	PHE	A	376	27.217	18.278	27.201	1.00 57.91	A
ATOM	2918	C	PHE	A	376	32.870	20.601	24.942	1.00 74.38	A
ATOM	2919	O	PHE	A	376	33.449	19.686	24.353	1.00 74.38	A
ATOM	2920	N	ARG	A	377	33.240	21.874	24.837	1.00100.66	A
ATOM	2921	CA	ARG	A	377	34.373	22.267	24.004	1.00100.66	A
ATOM	2922	CB	ARG	A	377	34.532	23.789	24.013	1.00127.11	A
ATOM	2923	CG	ARG	A	377	33.342	24.546	23.444	1.00127.11	A
ATOM	2924	CD	ARG	A	377	33.595	26.047	23.462	1.00127.11	A
ATOM	2925	NE	ARG	A	377	32.486	26.809	22.893	1.00127.11	A
ATOM	2926	CZ	ARG	A	377	32.472	28.134	22.780	1.00127.11	A
ATOM	2927	NH1	ARG	A	377	33.508	28.849	23.198	1.00127.11	A
ATOM	2928	NH2	ARG	A	377	31.423	28.747	22.248	1.00127.11	A
ATOM	2929	C	ARG	A	377	35.676	21.613	24.466	1.00100.66	A
ATOM	2930	O	ARG	A	377	36.444	21.101	23.651	1.00100.66	A
ATOM	2931	N	LYS	A	378	35.914	21.626	25.775	1.00114.97	A
ATOM	2932	CA	LYS	A	378	37.127	21.048	26.351	1.00114.97	A
ATOM	2933	CB	LYS	A	378	37.396	21.667	27.728	1.00131.02	A
ATOM	2934	CG	LYS	A	378	38.739	21.289	28.345	1.00131.02	A
ATOM	2935	CD	LYS	A	378	39.908	21.866	27.553	1.00131.02	A
ATOM	2936	CE	LYS	A	378	41.244	21.539	28.211	1.00131.02	A
ATOM	2937	NZ	LYS	A	378	42.406	22.107	27.467	1.00131.02	A
ATOM	2938	C	LYS	A	378	37.061	19.523	26.482	1.00114.97	A
ATOM	2939	O	LYS	A	378	37.970	18.821	26.036	1.00114.97	A
ATOM	2940	N	ILE	A	379	35.988	19.027	27.097	1.00 92.81	A
ATOM	2941	CA	ILE	A	379	35.775	17.591	27.314	1.00 92.81	A
ATOM	2942	CB	ILE	A	379	34.265	17.267	27.384	1.00 81.77	A
ATOM	2943	CG2	ILE	A	379	34.051	15.774	27.574	1.00 81.77	A
ATOM	2944	CG1	ILE	A	379	33.627	18.044	28.534	1.00 81.77	A
ATOM	2945	CD1	ILE	A	379	32.126	17.890	28.612	1.00 81.77	A
ATOM	2946	C	ILE	A	379	36.410	16.690	26.254	1.00 92.81	A
ATOM	2947	O	ILE	A	379	36.134	16.828	25.062	1.00 92.81	A
ATOM	2948	N	ARG	A	380	37.261	15.767	26.698	1.00111.06	A
ATOM	2949	CA	ARG	A	380	37.930	14.842	25.789	1.00111.06	A

FIGURE 25 CON'T

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ATOM   2950  CB  ARG A 380      39.002  14.035  26.530  1.00115.46      A
ATOM   2951  CG  ARG A 380      40.322  14.765  26.730  1.00115.46      A
ATOM   2952  CD  ARG A 380      41.429  13.795  27.137  1.00115.46      A
ATOM   2953  NE  ARG A 380      42.750  14.421  27.104  1.00115.46      A
ATOM   2954  CZ  ARG A 380      43.889  13.778  27.343  1.00115.46      A
ATOM   2955  NH1 ARG A 380      43.875  12.484  27.633  1.00115.46      A
ATOM   2956  NH2 ARG A 380      45.045  14.428  27.289  1.00115.46      A
ATOM   2957  C   ARG A 380      36.937  13.883  25.142  1.00111.06      A
ATOM   2958  O   ARG A 380      36.373  14.174  24.087  1.00111.06      A
ATOM   2959  N   GLU A 381      36.735  12.736  25.782  1.00 81.80      A
ATOM   2960  CA  GLU A 381      35.814  11.722  25.286  1.00 81.80      A
ATOM   2961  CB  GLU A 381      36.499  10.359  25.238  1.00109.22      A
ATOM   2962  CG  GLU A 381      36.798   9.811  26.627  1.00109.22      A
ATOM   2963  CD  GLU A 381      37.160   8.342  26.620  1.00109.22      A
ATOM   2964  OE1 GLU A 381      36.351   7.534  26.118  1.00109.22      A
ATOM   2965  OE2 GLU A 381      38.250   7.995  27.124  1.00109.22      A
ATOM   2966  C   GLU A 381      34.619  11.611  26.226  1.00 81.80      A
ATOM   2967  O   GLU A 381      34.671  12.036  27.380  1.00 81.80      A
ATOM   2968  N   ILE A 382      33.541  11.030  25.722  1.00 54.73      A
ATOM   2969  CA  ILE A 382      32.351  10.824  26.529  1.00 54.73      A
ATOM   2970  CB  ILE A 382      31.170  11.684  26.028  1.00 57.74      A
ATOM   2971  CG2 ILE A 382      29.906  11.352  26.817  1.00 57.74      A

ATOM   2972  CG1 ILE A 382      31.511  13.167  26.185  1.00 57.74      A
ATOM   2973  CD1 ILE A 382      30.405  14.104  25.745  1.00 57.74      A
ATOM   2974  C   ILE A 382      31.995   9.345  26.427  1.00 54.73      A
ATOM   2975  O   ILE A 382      31.445   8.903  25.428  1.00 54.73      A
ATOM   2976  N   PRO A 383      32.350   8.551  27.450  1.00 43.50      A
ATOM   2977  CD  PRO A 383      33.094   8.915  28.670  1.00 50.24      A
ATOM   2978  CA  PRO A 383      32.041   7.116  27.432  1.00 43.50      A
ATOM   2979  CB  PRO A 383      32.477   6.654  28.821  1.00 50.24      A
ATOM   2980  CG  PRO A 383      33.625   7.577  29.130  1.00 50.24      A
ATOM   2981  C   PRO A 383      30.538   6.898  27.191  1.00 43.50      A
ATOM   2982  O   PRO A 383      29.705   7.629  27.729  1.00 43.50      A
ATOM   2983  N   MSE A 384      30.214   5.884  26.393  1.00 58.26      A
ATOM   2984  CA  MSE A 384      28.830   5.562  26.050  1.00 58.26      A
ATOM   2985  CB  MSE A 384      28.656   5.580  24.531  1.00174.03      A
ATOM   2986  CG  MSE A 384      27.298   6.058  24.071  1.00174.03      A
ATOM   2987  SE  MSE A 384      27.115   7.952  24.377  1.00174.03      A
ATOM   2988  CE  MSE A 384      27.699   8.580  22.656  1.00174.03      A
ATOM   2989  C   MSE A 384      28.429   4.188  26.577  1.00 58.26      A
ATOM   2990  O   MSE A 384      29.040   3.182  26.231  1.00 58.26      A
ATOM   2991  N   PHE A 385      27.387   4.144  27.399  1.00 44.08      A
ATOM   2992  CA  PHE A 385      26.925   2.883  27.963  1.00 44.08      A
ATOM   2993  CB  PHE A 385      26.897   2.981  29.487  1.00 43.39      A
ATOM   2994  CG  PHE A 385      28.220   3.286  30.093  1.00 43.39      A
ATOM   2995  CD1 PHE A 385      29.180   2.279  30.252  1.00 43.39      A
ATOM   2996  CD2 PHE A 385      28.522   4.579  30.504  1.00 43.39      A
ATOM   2997  CE1 PHE A 385      30.423   2.563  30.813  1.00 43.39      A
ATOM   2998  CE2 PHE A 385      29.758   4.878  31.068  1.00 43.39      A
ATOM   2999  CZ  PHE A 385      30.715   3.865  31.223  1.00 43.39      A
ATOM   3000  C   PHE A 385      25.539   2.483  27.476  1.00 44.08      A
ATOM   3001  O   PHE A 385      24.614   3.298  27.478  1.00 44.08      A
ATOM   3002  N   ILE A 386      25.417   1.225  27.061  1.00 38.93      A
ATOM   3003  CA  ILE A 386      24.159   0.638  26.606  1.00 38.93      A
ATOM   3004  CB  ILE A 386      24.322  -0.164  25.295  1.00 45.03      A
ATOM   3005  CG2 ILE A 386      23.020  -0.893  24.961  1.00 45.03      A
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FIGURE 25 CON'T
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ATOM   3006  CG1 ILE A 386      24.791   0.759  24.164  1.00 45.03      A
ATOM   3007  CD1 ILE A 386      24.047   2.033  24.095  1.00 45.03      A
ATOM   3008  C   ILE A 386      23.805  -0.350  27.701  1.00 38.93      A
ATOM   3009  O   ILE A 386      24.476  -1.365  27.852  1.00 38.93      A
ATOM   3010  N   ILE A 387      22.760  -0.060  28.464  1.00 36.29      A
ATOM   3011  CA  ILE A 387      22.356  -0.925  29.568  1.00 36.29      A
ATOM   3012  CB  ILE A 387      22.175  -0.086  30.840  1.00 38.17      A
ATOM   3013  CG2 ILE A 387      21.760  -0.979  32.023  1.00 38.17      A
ATOM   3014  CG1 ILE A 387      23.499   0.633  31.130  1.00 38.17      A
ATOM   3015  CD1 ILE A 387      23.485   1.568  32.316  1.00 38.17      A
ATOM   3016  C   ILE A 387      21.081  -1.681  29.223  1.00 36.29      A
ATOM   3017  O   ILE A 387      20.003  -1.092  29.095  1.00 36.29      A
ATOM   3018  N   LEU A 388      21.215  -2.996  29.090  1.00 43.27      A
ATOM   3019  CA  LEU A 388      20.106  -3.850  28.703  1.00 43.27      A
ATOM   3020  CB  LEU A 388      20.537  -4.738  27.538  1.00 38.32      A
ATOM   3021  CG  LEU A 388      21.153  -4.011  26.333  1.00 38.32      A
ATOM   3022  CD1 LEU A 388      21.640  -5.036  25.277  1.00 38.32      A
ATOM   3023  CD2 LEU A 388      20.109  -3.058  25.752  1.00 38.32      A
ATOM   3024  C   LEU A 388      19.516  -4.728  29.796  1.00 43.27      A
ATOM   3025  O   LEU A 388      20.197  -5.563  30.389  1.00 43.27      A
ATOM   3026  N   ASP A 389      18.231  -4.538  30.042  1.00 49.60      A
ATOM   3027  CA  ASP A 389      17.533  -5.324  31.030  1.00 49.60      A
ATOM   3028  CB  ASP A 389      16.119  -4.790  31.185  1.00 45.78      A
ATOM   3029  CG  ASP A 389      15.357  -5.504  32.251  1.00 45.78      A
ATOM   3030  OD1 ASP A 389      15.977  -6.321  32.960  1.00 45.78      A
ATOM   3031  OD2 ASP A 389      14.144  -5.242  32.386  1.00 45.78      A
ATOM   3032  C   ASP A 389      17.512  -6.766  30.516  1.00 49.60      A
ATOM   3033  O   ASP A 389      16.870  -7.055  29.502  1.00 49.60      A
ATOM   3034  N   SER A 390      18.219  -7.659  31.208  1.00 56.04      A
ATOM   3035  CA  SER A 390      18.299  -9.056  30.794  1.00 56.04      A
ATOM   3036  CB  SER A 390      19.178  -9.861  31.757  1.00 40.57      A
ATOM   3037  OG  SER A 390      18.614  -9.872  33.058  1.00 40.57      A
ATOM   3038  C   SER A 390      16.932  -9.713  30.692  1.00 56.04      A
ATOM   3039  O   SER A 390      16.796 -10.764  30.073  1.00 56.04      A
ATOM   3040  N   GLY A 391      15.925  -9.098  31.302  1.00 60.83      A
ATOM   3041  CA  GLY A 391      14.585  -9.651  31.236  1.00 60.83      A
ATOM   3042  C   GLY A 391      13.949  -9.514  29.859  1.00 60.83      A
ATOM   3043  O   GLY A 391      13.041 -10.271  29.519  1.00 60.83      A
ATOM   3044  N   LEU A 392      14.420  -8.559  29.061  1.00 55.40      A
ATOM   3045  CA  LEU A 392      13.868  -8.345  27.724  1.00 55.40      A
ATOM   3046  CB  LEU A 392      14.343  -7.006  27.154  1.00 36.97      A
ATOM   3047  CG  LEU A 392      14.002  -5.708  27.896  1.00 36.97      A
ATOM   3048  CD1 LEU A 392      14.885  -4.596  27.350  1.00 36.97      A
ATOM   3049  CD2 LEU A 392      12.506  -5.368  27.742  1.00 36.97      A
ATOM   3050  C   LEU A 392      14.281  -9.454  26.755  1.00 55.40      A
ATOM   3051  O   LEU A 392      15.410  -9.947  26.808  1.00 55.40      A
ATOM   3052  N   LEU A 393      13.364  -9.839  25.868  1.00 60.39      A
ATOM   3053  CA  LEU A 393      13.661 -10.867  24.874  1.00 60.39      A
ATOM   3054  CB  LEU A 393      12.482 -11.044  23.914  1.00 55.91      A
ATOM   3055  CG  LEU A 393      11.209 -11.658  24.505  1.00 55.91      A
ATOM   3056  CD1 LEU A 393      10.057 -11.490  23.528  1.00 55.91      A
ATOM   3057  CD2 LEU A 393      11.447 -13.125  24.823  1.00 55.91      A
ATOM   3058  C   LEU A 393      14.891 -10.427  24.094  1.00 60.39      A
ATOM   3059  O   LEU A 393      15.143  -9.228  23.938  1.00 60.39      A
ATOM   3060  N   ALA A 394      15.658 -11.395  23.608  1.00 60.28      A
ATOM   3061  CA  ALA A 394      16.865 -11.101  22.847  1.00 60.28      A
ATOM   3062  CB  ALA A 394      17.460 -12.394  22.303  1.00 64.50      A
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FIGURE 25 CON'T
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ATOM   3063  C   ALA A 394      16.635 -10.112  21.701  1.00 60.28      A
ATOM   3064  O   ALA A 394      17.414  -9.177  21.523  1.00 60.28      A
ATOM   3065  N   ASP A 395      15.570 -10.317  20.929  1.00 55.46      A
ATOM   3066  CA  ASP A 395      15.279  -9.443  19.796  1.00 55.46      A
ATOM   3067  CB  ASP A 395      14.128 -10.027  18.949  1.00 69.32      A
ATOM   3068  CG  ASP A 395      12.777  -9.939  19.632  1.00 69.32      A
ATOM   3069  OD1 ASP A 395      12.217  -8.825  19.709  1.00 69.32      A
ATOM   3070  OD2 ASP A 395      12.264 -10.988  20.085  1.00 69.32      A
ATOM   3071  C   ASP A 395      14.985  -7.996  20.200  1.00 55.46      A
ATOM   3072  O   ASP A 395      15.308  -7.065  19.466  1.00 55.46      A
ATOM   3073  N   ILE A 396      14.366  -7.805  21.359  1.00 47.75      A
ATOM   3074  CA  ILE A 396      14.087  -6.457  21.835  1.00 47.75      A
ATOM   3075  CB  ILE A 396      13.179  -6.472  23.073  1.00 47.69      A
ATOM   3076  CG2 ILE A 396      12.956  -5.042  23.554  1.00 47.69      A
ATOM   3077  CG1 ILE A 396      11.849  -7.161  22.746  1.00 47.69      A
ATOM   3078  CD1 ILE A 396      11.006  -6.430  21.721  1.00 47.69      A
ATOM   3079  C   ILE A 396      15.439  -5.825  22.220  1.00 47.75      A
ATOM   3080  O   ILE A 396      15.713  -4.664  21.906  1.00 47.75      A
ATOM   3081  N   GLN A 397      16.280  -6.611  22.888  1.00 48.02      A
ATOM   3082  CA  GLN A 397      17.603  -6.148  23.295  1.00 48.02      A
ATOM   3083  CB  GLN A 397      18.369  -7.256  24.029  1.00 48.61      A
ATOM   3084  CG  GLN A 397      17.952  -7.448  25.475  1.00 48.61      A
ATOM   3085  CD  GLN A 397      18.797  -8.491  26.195  1.00 48.61      A
ATOM   3086  OE1 GLN A 397      20.023  -8.516  26.070  1.00 48.61      A
ATOM   3087  NE2 GLN A 397      18.147  -9.346  26.957  1.00 48.61      A
ATOM   3088  C   GLN A 397      18.415  -5.677  22.095  1.00 48.02      A
ATOM   3089  O   GLN A 397      19.048  -4.630  22.155  1.00 48.02      A
ATOM   3090  N   ASN A 398      18.396  -6.442  21.004  1.00 58.81      A
ATOM   3091  CA  ASN A 398      19.147  -6.057  19.807  1.00 58.81      A
ATOM   3092  CB  ASN A 398      19.142  -7.189  18.779  1.00110.12      A
ATOM   3093  CG  ASN A 398      19.876  -8.418  19.268  1.00110.12      A
ATOM   3094  OD1 ASN A 398      21.016  -8.331  19.726  1.00110.12      A
ATOM   3095  ND2 ASN A 398      19.230  -9.575  19.168  1.00110.12      A
ATOM   3096  C   ASN A 398      18.578  -4.792  19.176  1.00 58.81      A
ATOM   3097  O   ASN A 398      19.320  -3.925  18.714  1.00 58.81      A
ATOM   3098  N   PHE A 399      17.256  -4.698  19.147  1.00 52.07      A
ATOM   3099  CA  PHE A 399      16.583  -3.530  18.586  1.00 52.07      A

ATOM   3100  CB  PHE A 399      15.068  -3.680  18.757  1.00 70.91      A
ATOM   3101  CG  PHE A 399      14.275  -2.502  18.267  1.00 70.91      A
ATOM   3102  CD1 PHE A 399      14.162  -2.237  16.908  1.00 70.91      A
ATOM   3103  CD2 PHE A 399      13.625  -1.664  19.169  1.00 70.91      A
ATOM   3104  CE1 PHE A 399      13.411  -1.156  16.451  1.00 70.91      A
ATOM   3105  CE2 PHE A 399      12.871  -0.579  18.721  1.00 70.91      A
ATOM   3106  CZ  PHE A 399      12.765  -0.327  17.358  1.00 70.91      A
ATOM   3107  C   PHE A 399      17.070  -2.270  19.312  1.00 52.07      A
ATOM   3108  O   PHE A 399      17.555  -1.324  18.686  1.00 52.07      A
ATOM   3109  N   ALA A 400      16.940  -2.276  20.637  1.00 49.37      A
ATOM   3110  CA  ALA A 400      17.357  -1.149  21.471  1.00 49.37      A
ATOM   3111  CB  ALA A 400      17.125  -1.478  22.945  1.00 38.64      A
ATOM   3112  C   ALA A 400      18.811  -0.716  21.260  1.00 49.37      A
ATOM   3113  O   ALA A 400      19.081   0.468  21.040  1.00 49.37      A
ATOM   3114  N   THR A 401      19.754  -1.651  21.315  1.00 50.15      A
ATOM   3115  CA  THR A 401      21.140  -1.245  21.140  1.00 50.15      A
ATOM   3116  CB  THR A 401      22.139  -2.419  21.318  1.00 55.89      A
ATOM   3117  OG1 THR A 401      22.499  -2.940  20.038  1.00 55.89      A
ATOM   3118  CG2 THR A 401      21.545  -3.517  22.159  1.00 55.89      A
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FIGURE 25 CON'T

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ATOM   3119  C   THR A 401      21.328  -0.608  19.759  1.00 50.15      A
ATOM   3120  O   THR A 401      22.097   0.349  19.609  1.00 50.15      A
ATOM   3121  N   ASN A 402      20.626  -1.118  18.747  1.00 54.40      A
ATOM   3122  CA  ASN A 402      20.755  -0.525  17.421  1.00 54.40      A
ATOM   3123  CB  ASN A 402      20.121  -1.416  16.345  1.00 77.17      A
ATOM   3124  CG  ASN A 402      20.976  -2.635  16.018  1.00 77.17      A
ATOM   3125  OD1 ASN A 402      22.208  -2.583  16.088  1.00 77.17      A
ATOM   3126  ND2 ASN A 402      20.327  -3.732  15.640  1.00 77.17      A
ATOM   3127  C   ASN A 402      20.132   0.868  17.407  1.00 54.40      A
ATOM   3128  O   ASN A 402      20.646   1.769  16.742  1.00 54.40      A
ATOM   3129  N   GLU A 403      19.031   1.050  18.135  1.00 49.70      A
ATOM   3130  CA  GLU A 403      18.398   2.367  18.205  1.00 49.70      A
ATOM   3131  CB  GLU A 403      17.073   2.321  18.985  1.00 49.89      A
ATOM   3132  CG  GLU A 403      15.827   2.069  18.156  1.00 49.89      A
ATOM   3133  CD  GLU A 403      15.624   3.095  17.044  1.00 49.89      A
ATOM   3134  OE1 GLU A 403      15.560   4.317  17.328  1.00 49.89      A
ATOM   3135  OE2 GLU A 403      15.527   2.661  15.877  1.00 49.89      A
ATOM   3136  C   GLU A 403      19.338   3.325  18.928  1.00 49.70      A
ATOM   3137  O   GLU A 403      19.517   4.468  18.514  1.00 49.70      A
ATOM   3138  N   PHE A 404      19.930   2.854  20.022  1.00 37.64      A
ATOM   3139  CA  PHE A 404      20.839   3.694  20.808  1.00 37.64      A
ATOM   3140  CB  PHE A 404      21.262   2.980  22.108  1.00 42.21      A
ATOM   3141  CG  PHE A 404      20.122   2.683  23.050  1.00 42.21      A
ATOM   3142  CD1 PHE A 404      19.042   3.555  23.162  1.00 42.21      A
ATOM   3143  CD2 PHE A 404      20.170   1.571  23.889  1.00 42.21      A
ATOM   3144  CE1 PHE A 404      18.029   3.330  24.100  1.00 42.21      A
ATOM   3145  CE2 PHE A 404      19.163   1.338  24.831  1.00 42.21      A
ATOM   3146  CZ  PHE A 404      18.093   2.219  24.937  1.00 42.21      A
ATOM   3147  C   PHE A 404      22.083   4.070  20.013  1.00 37.64      A
ATOM   3148  O   PHE A 404      22.570   5.186  20.111  1.00 37.64      A
ATOM   3149  N   ARG A 405      22.607   3.122  19.243  1.00 47.85      A
ATOM   3150  CA  ARG A 405      23.791   3.376  18.432  1.00 47.85      A
ATOM   3151  CB  ARG A 405      24.184   2.114  17.666  1.00 54.53      A
ATOM   3152  CG  ARG A 405      24.918   1.121  18.537  1.00 54.53      A
ATOM   3153  CD  ARG A 405      25.170  -0.193  17.835  1.00 54.53      A
ATOM   3154  NE  ARG A 405      26.055  -1.022  18.642  1.00 54.53      A
ATOM   3155  CZ  ARG A 405      26.160  -2.339  18.536  1.00 54.53      A
ATOM   3156  NH1 ARG A 405      25.430  -2.998  17.653  1.00 54.53      A
ATOM   3157  NH2 ARG A 405      27.001  -2.997  19.322  1.00 54.53      A
ATOM   3158  C   ARG A 405      23.562   4.524  17.460  1.00 47.85      A
ATOM   3159  O   ARG A 405      24.430   5.370  17.276  1.00 47.85      A
ATOM   3160  N   GLU A 406      22.386   4.559  16.844  1.00 45.39      A
ATOM   3161  CA  GLU A 406      22.081   5.623  15.898  1.00 45.39      A
ATOM   3162  CB  GLU A 406      20.885   5.241  15.022  1.00 63.52      A
ATOM   3163  CG  GLU A 406      21.147   4.064  14.108  1.00 63.52      A
ATOM   3164  CD  GLU A 406      22.394   4.256  13.260  1.00 63.52      A
ATOM   3165  OE1 GLU A 406      22.572   5.354  12.687  1.00 63.52      A
ATOM   3166  OE2 GLU A 406      23.197   3.307  13.162  1.00 63.52      A
ATOM   3167  C   GLU A 406      21.791   6.920  16.628  1.00 45.39      A
ATOM   3168  O   GLU A 406      22.093   7.998  16.129  1.00 45.39      A
ATOM   3169  N   LEU A 407      21.204   6.819  17.817  1.00 51.19      A
ATOM   3170  CA  LEU A 407      20.896   8.015  18.586  1.00 51.19      A
ATOM   3171  CB  LEU A 407      20.106   7.651  19.844  1.00 55.82      A
ATOM   3172  CG  LEU A 407      19.425   8.803  20.586  1.00 55.82      A
ATOM   3173  CD1 LEU A 407      18.523   8.239  21.659  1.00 55.82      A
ATOM   3174  CD2 LEU A 407      20.457   9.721  21.194  1.00 55.82      A
ATOM   3175  C   LEU A 407      22.192   8.733  18.959  1.00 51.19      A
```

FIGURE 25 CON'T

```
ATOM   3176  O   LEU A 407      22.280   9.956  18.859  1.00 51.19      A
ATOM   3177  N   VAL A 408      23.204   7.982  19.379  1.00 54.33      A
ATOM   3178  CA  VAL A 408      24.465   8.614  19.747  1.00 54.33      A
ATOM   3179  CB  VAL A 408      25.446   7.612  20.411  1.00 69.32      A
ATOM   3180  CG1 VAL A 408      24.853   7.098  21.706  1.00 69.32      A
ATOM   3181  CG2 VAL A 408      25.749   6.460  19.468  1.00 69.32      A
ATOM   3182  C   VAL A 408      25.147   9.262  18.545  1.00 54.33      A
ATOM   3183  O   VAL A 408      25.741  10.334  18.670  1.00 54.33      A
ATOM   3184  N   LYS A 409      25.064   8.625  17.382  1.00 55.85      A
ATOM   3185  CA  LYS A 409      25.677   9.191  16.185  1.00 55.85      A
ATOM   3186  CB  LYS A 409      25.433   8.287  14.979  1.00 68.43      A
ATOM   3187  CG  LYS A 409      26.205   6.986  15.053  1.00 68.43      A
ATOM   3188  CD  LYS A 409      25.832   6.029  13.940  1.00 68.43      A
ATOM   3189  CE  LYS A 409      26.575   4.710  14.106  1.00 68.43      A
ATOM   3190  NZ  LYS A 409      26.108   3.662  13.151  1.00 68.43      A
ATOM   3191  C   LYS A 409      25.139  10.591  15.915  1.00 55.85      A
ATOM   3192  O   LYS A 409      25.917  11.531  15.766  1.00 55.85      A
ATOM   3193  N   SER A 410      23.817  10.748  15.868  1.00 59.15      A
ATOM   3194  CA  SER A 410      23.254  12.070  15.620  1.00 59.15      A
ATOM   3195  CB  SER A 410      21.739  11.995  15.413  1.00 72.56      A
ATOM   3196  OG  SER A 410      21.083  11.594  16.597  1.00 72.56      A
ATOM   3197  C   SER A 410      23.584  12.963  16.816  1.00 59.15      A
ATOM   3198  O   SER A 410      23.730  14.182  16.682  1.00 59.15      A
ATOM   3199  N   MSE A 411      23.695  12.344  17.985  1.00 63.76      A
ATOM   3200  CA  MSE A 411      24.044  13.059  19.207  1.00 63.76      A
ATOM   3201  CB  MSE A 411      24.321  12.058  20.327  1.00100.84      A
ATOM   3202  CG  MSE A 411      23.146  11.807  21.223  1.00100.84      A
ATOM   3203  SE  MSE A 411      22.889  13.373  22.260  1.00100.84      A
ATOM   3204  CE  MSE A 411      24.121  12.935  23.679  1.00100.84      A
ATOM   3205  C   MSE A 411      25.302  13.885  18.938  1.00 63.76      A
ATOM   3206  O   MSE A 411      25.502  14.956  19.514  1.00 63.76      A
ATOM   3207  N   TYR A 412      26.144  13.364  18.052  1.00 85.83      A
ATOM   3208  CA  TYR A 412      27.377  14.033  17.674  1.00 85.83      A
ATOM   3209  CB  TYR A 412      28.501  13.008  17.512  1.00113.02      A
ATOM   3210  CG  TYR A 412      28.851  12.306  18.805  1.00113.02      A
ATOM   3211  CD1 TYR A 412      29.215  13.036  19.935  1.00113.02      A
ATOM   3212  CE1 TYR A 412      29.534  12.401  21.133  1.00113.02      A
ATOM   3213  CD2 TYR A 412      28.815  10.915  18.903  1.00113.02      A
ATOM   3214  CE2 TYR A 412      29.133  10.268  20.099  1.00113.02      A
ATOM   3215  CZ  TYR A 412      29.492  11.020  21.210  1.00113.02      A
ATOM   3216  OH  TYR A 412      29.811  10.397  22.396  1.00113.02      A
ATOM   3217  C   TYR A 412      27.164  14.809  16.383  1.00 85.83      A
ATOM   3218  O   TYR A 412      27.591  14.390  15.304  1.00 85.83      A
ATOM   3219  N   TYR A 413      26.473  15.936  16.529  1.00 87.35      A
ATOM   3220  CA  TYR A 413      26.150  16.866  15.451  1.00 87.35      A
ATOM   3221  CB  TYR A 413      26.379  18.294  15.955  1.00 83.41      A
ATOM   3222  CG  TYR A 413      26.617  18.343  17.449  1.00 83.41      A
ATOM   3223  CD1 TYR A 413      25.598  18.009  18.344  1.00 83.41      A
ATOM   3224  CE1 TYR A 413      25.836  17.940  19.716  1.00 83.41      A
ATOM   3225  CD2 TYR A 413      27.887  18.624  17.968  1.00 83.41      A
ATOM   3226  CE2 TYR A 413      28.136  18.559  19.345  1.00 83.41      A
ATOM   3227  CZ  TYR A 413      27.102  18.210  20.209  1.00 83.41      A

ATOM   3228  OH  TYR A 413      27.329  18.094  21.560  1.00 83.41      A
ATOM   3229  C   TYR A 413      26.966  16.625  14.180  1.00 87.35      A
ATOM   3230  O   TYR A 413      26.641  15.750  13.375  1.00 87.35      A
ATOM   3231  N   GLU A 443      32.228   2.350  23.459  1.00 66.73      A
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FIGURE 25 CON'T

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ATOM   3232  CA  GLU A 443      30.888   1.809  23.680  1.00 66.73      A
ATOM   3233  CB  GLU A 443      30.221   1.471  22.348  1.00 80.66      A
ATOM   3234  CG  GLU A 443      28.779   0.997  22.488  1.00 80.66      A
ATOM   3235  CD  GLU A 443      28.366   0.036  21.385  1.00 80.66      A
ATOM   3236  OE1 GLU A 443      28.796  -1.137  21.427  1.00 80.66      A
ATOM   3237  OE2 GLU A 443      27.619   0.452  20.474  1.00 80.66      A
ATOM   3238  C   GLU A 443      30.938   0.548  24.537  1.00 66.73      A
ATOM   3239  O   GLU A 443      31.601  -0.428  24.186  1.00 66.73      A
ATOM   3240  N   LYS A 444      30.229   0.560  25.656  1.00 47.77      A
ATOM   3241  CA  LYS A 444      30.225  -0.600  26.532  1.00 47.77      A
ATOM   3242  CB  LYS A 444      30.852  -0.244  27.885  1.00 86.81      A
ATOM   3243  CG  LYS A 444      31.656  -1.376  28.528  1.00 86.81      A
ATOM   3244  CD  LYS A 444      30.787  -2.580  28.867  1.00 86.81      A
ATOM   3245  CE  LYS A 444      31.609  -3.762  29.396  1.00 86.81      A
ATOM   3246  NZ  LYS A 444      32.471  -4.435  28.367  1.00 86.81      A
ATOM   3247  C   LYS A 444      28.798  -1.084  26.722  1.00 47.77      A
ATOM   3248  O   LYS A 444      27.926  -0.317  27.142  1.00 47.77      A
ATOM   3249  N   VAL A 445      28.559  -2.353  26.398  1.00 48.00      A
ATOM   3250  CA  VAL A 445      27.238  -2.948  26.543  1.00 48.00      A
ATOM   3251  CB  VAL A 445      26.908  -3.893  25.375  1.00 44.91      A
ATOM   3252  CG1 VAL A 445      25.528  -4.525  25.593  1.00 44.91      A
ATOM   3253  CG2 VAL A 445      26.935  -3.125  24.060  1.00 44.91      A
ATOM   3254  C   VAL A 445      27.148  -3.744  27.839  1.00 48.00      A
ATOM   3255  O   VAL A 445      27.938  -4.663  28.079  1.00 48.00      A
ATOM   3256  N   ILE A 446      26.185  -3.391  28.680  1.00 43.39      A
ATOM   3257  CA  ILE A 446      26.018  -4.092  29.934  1.00 43.39      A
ATOM   3258  CB  ILE A 446      26.253  -3.140  31.110  1.00 50.34      A
ATOM   3259  CG2 ILE A 446      25.991  -3.850  32.426  1.00 50.34      A
ATOM   3260  CG1 ILE A 446      27.698  -2.632  31.059  1.00 50.34      A
ATOM   3261  CD1 ILE A 446      27.976  -1.466  31.997  1.00 50.34      A
ATOM   3262  C   ILE A 446      24.628  -4.705  30.000  1.00 43.39      A
ATOM   3263  O   ILE A 446      23.624  -4.023  29.791  1.00 43.39      A
ATOM   3264  N   THR A 447      24.575  -5.999  30.285  1.00 45.08      A
ATOM   3265  CA  THR A 447      23.308  -6.715  30.370  1.00 45.08      A
ATOM   3266  CB  THR A 447      23.246  -7.840  29.316  1.00 46.71      A
ATOM   3267  OG1 THR A 447      23.499  -7.292  28.015  1.00 46.71      A
ATOM   3268  CG2 THR A 447      21.864  -8.513  29.324  1.00 46.71      A
ATOM   3269  C   THR A 447      23.117  -7.338  31.750  1.00 45.08      A
ATOM   3270  O   THR A 447      23.868  -8.222  32.133  1.00 45.08      A
ATOM   3271  N   GLU A 448      22.108  -6.888  32.490  1.00 47.89      A
ATOM   3272  CA  GLU A 448      21.841  -7.432  33.821  1.00 47.89      A
ATOM   3273  CB  GLU A 448      22.561  -6.614  34.902  1.00 48.58      A
ATOM   3274  CG  GLU A 448      24.084  -6.603  34.832  1.00 48.58      A
ATOM   3275  CD  GLU A 448      24.708  -7.982  34.994  1.00 48.58      A
ATOM   3276  OE1 GLU A 448      24.188  -8.803  35.790  1.00 48.58      A
ATOM   3277  OE2 GLU A 448      25.733  -8.240  34.330  1.00 48.58      A
ATOM   3278  C   GLU A 448      20.348  -7.434  34.122  1.00 47.89      A
ATOM   3279  O   GLU A 448      19.547  -6.879  33.366  1.00 47.89      A
ATOM   3280  N   ASP A 449      19.983  -8.053  35.240  1.00 50.32      A
ATOM   3281  CA  ASP A 449      18.595  -8.135  35.664  1.00 50.32      A
ATOM   3282  CB  ASP A 449      18.410  -9.334  36.598  1.00 66.69      A
ATOM   3283  CG  ASP A 449      16.969  -9.512  37.051  1.00 66.69      A
ATOM   3284  OD1 ASP A 449      16.116  -8.655  36.716  1.00 66.69      A
ATOM   3285  OD2 ASP A 449      16.697 -10.516  37.751  1.00 66.69      A
ATOM   3286  C   ASP A 449      18.195  -6.847  36.378  1.00 50.32      A
ATOM   3287  O   ASP A 449      18.244  -6.758  37.610  1.00 50.32      A
ATOM   3288  N   LEU A 450      17.791  -5.855  35.592  1.00 56.84      A
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FIGURE 25 CON'T

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ATOM   3289  CA  LEU A 450      17.391  -4.555  36.118  1.00 56.84      A
ATOM   3290  CB  LEU A 450      17.055  -3.610  34.958  1.00 46.05      A
ATOM   3291  CG  LEU A 450      18.164  -2.655  34.477  1.00 46.05      A
ATOM   3292  CD1 LEU A 450      19.552  -3.248  34.718  1.00 46.05      A
ATOM   3293  CD2 LEU A 450      17.941  -2.336  33.006  1.00 46.05      A
ATOM   3294  C   LEU A 450      16.229  -4.601  37.104  1.00 56.84      A
ATOM   3295  O   LEU A 450      15.948  -3.610  37.776  1.00 56.84      A
ATOM   3296  N   ASN A 451      15.554  -5.743  37.200  1.00 62.74      A
ATOM   3297  CA  ASN A 451      14.431  -5.851  38.123  1.00 62.74      A
ATOM   3298  CB  ASN A 451      13.287  -6.642  37.485  1.00 81.07      A
ATOM   3299  CG  ASN A 451      12.000  -6.545  38.282  1.00 81.07      A
ATOM   3300  OD1 ASN A 451      11.582  -5.451  38.675  1.00 81.07      A
ATOM   3301  ND2 ASN A 451      11.361  -7.686  38.521  1.00 81.07      A
ATOM   3302  C   ASN A 451      14.826  -6.488  39.450  1.00 62.74      A
ATOM   3303  O   ASN A 451      13.978  -6.951  40.212  1.00 62.74      A
ATOM   3304  N   SER A 452      16.123  -6.512  39.723  1.00 55.07      A
ATOM   3305  CA  SER A 452      16.626  -7.073  40.968  1.00 55.07      A
ATOM   3306  CB  SER A 452      17.250  -8.446  40.718  1.00 56.63      A
ATOM   3307  OG  SER A 452      18.399  -8.345  39.903  1.00 56.63      A
ATOM   3308  C   SER A 452      17.670  -6.111  41.526  1.00 55.07      A
ATOM   3309  O   SER A 452      18.385  -5.450  40.774  1.00 55.07      A
ATOM   3310  N   ASP A 453      17.749  -6.019  42.845  1.00 61.74      A
ATOM   3311  CA  ASP A 453      18.706  -5.119  43.467  1.00 61.74      A
ATOM   3312  CB  ASP A 453      18.484  -5.081  44.981  1.00 86.73      A
ATOM   3313  CG  ASP A 453      17.188  -4.384  45.356  1.00 86.73      A
ATOM   3314  OD1 ASP A 453      16.888  -4.279  46.566  1.00 86.73      A
ATOM   3315  OD2 ASP A 453      16.469  -3.939  44.435  1.00 86.73      A
ATOM   3316  C   ASP A 453      20.133  -5.528  43.144  1.00 61.74      A
ATOM   3317  O   ASP A 453      21.013  -4.683  43.009  1.00 61.74      A
ATOM   3318  N   LYS A 454      20.350  -6.828  42.993  1.00 52.02      A
ATOM   3319  CA  LYS A 454      21.676  -7.360  42.685  1.00 52.02      A
ATOM   3320  CB  LYS A 454      21.673  -8.887  42.818  1.00126.78      A
ATOM   3321  CG  LYS A 454      20.631  -9.439  43.785  1.00126.78      A
ATOM   3322  CD  LYS A 454      19.233  -9.396  43.175  1.00126.78      A
ATOM   3323  CE  LYS A 454      18.173  -9.896  44.141  1.00126.78      A
ATOM   3324  NZ  LYS A 454      18.061  -9.024  45.340  1.00126.78      A
ATOM   3325  C   LYS A 454      22.109  -6.975  41.266  1.00 52.02      A
ATOM   3326  O   LYS A 454      23.288  -6.717  41.009  1.00 52.02      A
ATOM   3327  N   GLY A 455      21.154  -6.954  40.342  1.00 46.36      A
ATOM   3328  CA  GLY A 455      21.477  -6.599  38.970  1.00 46.36      A
ATOM   3329  C   GLY A 455      21.888  -5.138  38.895  1.00 46.36      A
ATOM   3330  O   GLY A 455      22.899  -4.788  38.277  1.00 46.36      A
ATOM   3331  N   ILE A 456      21.098  -4.290  39.544  1.00 53.41      A
ATOM   3332  CA  ILE A 456      21.365  -2.867  39.560  1.00 53.41      A
ATOM   3333  CB  ILE A 456      20.267  -2.119  40.333  1.00 42.96      A
ATOM   3334  CG2 ILE A 456      20.658  -0.643  40.515  1.00 42.96      A
ATOM   3335  CG1 ILE A 456      18.945  -2.253  39.562  1.00 42.96      A
ATOM   3336  CD1 ILE A 456      17.736  -1.670  40.260  1.00 42.96      A
ATOM   3337  C   ILE A 456      22.735  -2.595  40.163  1.00 53.41      A
ATOM   3338  O   ILE A 456      23.520  -1.840  39.591  1.00 53.41      A
ATOM   3339  N   ILE A 457      23.035  -3.224  41.299  1.00 59.64      A
ATOM   3340  CA  ILE A 457      24.341  -3.041  41.929  1.00 59.64      A
ATOM   3341  CB  ILE A 457      24.500  -3.931  43.192  1.00 70.44      A
ATOM   3342  CG2 ILE A 457      25.931  -3.884  43.695  1.00 70.44      A
ATOM   3343  CG1 ILE A 457      23.568  -3.441  44.300  1.00 70.44      A
ATOM   3344  CD1 ILE A 457      23.591  -4.315  45.537  1.00 70.44      A
ATOM   3345  C   ILE A 457      25.456  -3.371  40.933  1.00 59.64      A
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FIGURE 25 CON'T

```
ATOM   3346  O   ILE A 457      26.413  -2.616  40.805  1.00 59.64      A
ATOM   3347  N   GLU A 458      25.325  -4.490  40.223  1.00 44.35      A
ATOM   3348  CA  GLU A 458      26.329  -4.902  39.233  1.00 44.35      A
ATOM   3349  CB  GLU A 458      25.943  -6.244  38.604  1.00 77.66      A
ATOM   3350  CG  GLU A 458      26.894  -7.404  38.901  1.00 77.66      A
ATOM   3351  CD  GLU A 458      28.335  -7.136  38.476  1.00 77.66      A
ATOM   3352  OE1 GLU A 458      29.066  -6.476  39.240  1.00 77.66      A
ATOM   3353  OE2 GLU A 458      28.739  -7.577  37.378  1.00 77.66      A
ATOM   3354  C   GLU A 458      26.497  -3.854  38.122  1.00 44.35      A
ATOM   3355  O   GLU A 458      27.614  -3.598  37.672  1.00 44.35      A

ATOM   3356  N   VAL A 459      25.392  -3.256  37.677  1.00 40.06      A
ATOM   3357  CA  VAL A 459      25.453  -2.237  36.624  1.00 40.06      A
ATOM   3358  CB  VAL A 459      24.043  -1.675  36.268  1.00 38.40      A
ATOM   3359  CG1 VAL A 459      24.173  -0.545  35.234  1.00 38.40      A
ATOM   3360  CG2 VAL A 459      23.162  -2.786  35.713  1.00 38.40      A
ATOM   3361  C   VAL A 459      26.326  -1.071  37.077  1.00 40.06      A
ATOM   3362  O   VAL A 459      27.297  -0.708  36.409  1.00 40.06      A
ATOM   3363  N   VAL A 460      25.949  -0.492  38.212  1.00 44.57      A
ATOM   3364  CA  VAL A 460      26.648   0.633  38.812  1.00 44.57      A
ATOM   3365  CB  VAL A 460      26.020   0.959  40.184  1.00 43.98      A
ATOM   3366  CG1 VAL A 460      26.690   2.184  40.816  1.00 43.98      A
ATOM   3367  CG2 VAL A 460      24.542   1.205  40.004  1.00 43.98      A
ATOM   3368  C   VAL A 460      28.147   0.349  38.964  1.00 44.57      A
ATOM   3369  O   VAL A 460      28.976   1.173  38.583  1.00 44.57      A
ATOM   3370  N   GLU A 461      28.488  -0.825  39.491  1.00 47.44      A
ATOM   3371  CA  GLU A 461      29.889  -1.209  39.672  1.00 47.44      A
ATOM   3372  CB  GLU A 461      29.988  -2.578  40.349  1.00 98.43      A
ATOM   3373  CG  GLU A 461      29.828  -2.551  41.857  1.00 98.43      A
ATOM   3374  CD  GLU A 461      29.867  -3.941  42.467  1.00 98.43      A
ATOM   3375  OE1 GLU A 461      30.758  -4.732  42.090  1.00 98.43      A
ATOM   3376  OE2 GLU A 461      29.013  -4.242  43.326  1.00 98.43      A
ATOM   3377  C   GLU A 461      30.631  -1.250  38.343  1.00 47.44      A
ATOM   3378  O   GLU A 461      31.739  -0.721  38.223  1.00 47.44      A
ATOM   3379  N   GLN A 462      30.025  -1.884  37.345  1.00 44.62      A
ATOM   3380  CA  GLN A 462      30.647  -1.968  36.025  1.00 44.62      A
ATOM   3381  CB  GLN A 462      29.803  -2.824  35.069  1.00 80.21      A
ATOM   3382  CG  GLN A 462      29.788  -4.317  35.380  1.00 80.21      A
ATOM   3383  CD  GLN A 462      29.154  -5.144  34.262  1.00 80.21      A
ATOM   3384  OE1 GLN A 462      29.584  -5.085  33.106  1.00 80.21      A
ATOM   3385  NE2 GLN A 462      28.133  -5.926  34.605  1.00 80.21      A
ATOM   3386  C   GLN A 462      30.824  -0.572  35.430  1.00 44.62      A
ATOM   3387  O   GLN A 462      31.884  -0.252  34.885  1.00 44.62      A
ATOM   3388  N   VAL A 463      29.795   0.267  35.537  1.00 47.32      A
ATOM   3389  CA  VAL A 463      29.911   1.611  34.985  1.00 47.32      A
ATOM   3390  CB  VAL A 463      28.556   2.380  34.980  1.00 38.58      A
ATOM   3391  CG1 VAL A 463      28.775   3.792  34.482  1.00 38.58      A
ATOM   3392  CG2 VAL A 463      27.546   1.677  34.090  1.00 38.58      A
ATOM   3393  C   VAL A 463      30.941   2.450  35.752  1.00 47.32      A
ATOM   3394  O   VAL A 463      31.741   3.147  35.134  1.00 47.32      A
ATOM   3395  N   SER A 464      30.921   2.386  37.085  1.00 48.80      A
ATOM   3396  CA  SER A 464      31.866   3.171  37.883  1.00 48.80      A
ATOM   3397  CB  SER A 464      31.666   2.923  39.374  1.00 71.18      A
ATOM   3398  OG  SER A 464      32.154   1.651  39.735  1.00 71.18      A
ATOM   3399  C   SER A 464      33.288   2.810  37.495  1.00 48.80      A
ATOM   3400  O   SER A 464      34.163   3.674  37.415  1.00 48.80      A
ATOM   3401  N   SER A 465      33.508   1.526  37.236  1.00 54.68      A
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ATOM	3402	CA	SER	A	465	34.822	1.045	36.838	1.00	54.68	A
ATOM	3403	CB	SER	A	465	34.791	-0.477	36.685	1.00	66.14	A
ATOM	3404	OG	SER	A	465	35.994	-0.943	36.107	1.00	66.14	A
ATOM	3405	C	SER	A	465	35.313	1.682	35.533	1.00	54.68	A
ATOM	3406	O	SER	A	465	36.501	1.976	35.388	1.00	54.68	A
ATOM	3407	N	PHE	A	466	34.405	1.884	34.582	1.00	44.49	A
ATOM	3408	CA	PHE	A	466	34.764	2.492	33.294	1.00	44.49	A
ATOM	3409	CB	PHE	A	466	33.807	2.040	32.187	1.00	58.64	A
ATOM	3410	CG	PHE	A	466	34.007	0.631	31.749	1.00	58.64	A
ATOM	3411	CD1	PHE	A	466	33.524	-0.425	32.515	1.00	58.64	A
ATOM	3412	CD2	PHE	A	466	34.694	0.353	30.570	1.00	58.64	A
ATOM	3413	CE1	PHE	A	466	33.723	-1.750	32.116	1.00	58.64	A
ATOM	3414	CE2	PHE	A	466	34.899	-0.960	30.161	1.00	58.64	A
ATOM	3415	CZ	PHE	A	466	34.411	-2.018	30.939	1.00	58.64	A
ATOM	3416	C	PHE	A	466	34.745	4.015	33.316	1.00	44.49	A
ATOM	3417	O	PHE	A	466	35.256	4.647	32.394	1.00	44.49	A
ATOM	3418	N	MSE	A	467	34.152	4.597	34.355	1.00	42.37	A
ATOM	3419	CA	MSE	A	467	34.033	6.053	34.468	1.00	42.37	A
ATOM	3420	CB	MSE	A	467	32.664	6.437	35.042	1.00	42.50	A
ATOM	3421	CG	MSE	A	467	31.524	6.466	34.044	1.00	42.50	A
ATOM	3422	SE	MSE	A	467	31.884	7.652	32.579	1.00	42.50	A
ATOM	3423	CE	MSE	A	467	31.829	9.324	33.526	1.00	42.50	A
ATOM	3424	C	MSE	A	467	35.092	6.751	35.321	1.00	42.37	A
ATOM	3425	O	MSE	A	467	35.136	7.978	35.352	1.00	42.37	A
ATOM	3426	N	LYS	A	468	35.913	5.993	36.036	1.00	42.40	A
ATOM	3427	CA	LYS	A	468	36.927	6.622	36.877	1.00	42.40	A
ATOM	3428	CB	LYS	A	468	37.738	5.572	37.654	1.00	74.83	A
ATOM	3429	CG	LYS	A	468	38.409	4.495	36.813	1.00	74.83	A
ATOM	3430	CD	LYS	A	468	39.342	3.654	37.689	1.00	74.83	A
ATOM	3431	CE	LYS	A	468	39.923	2.453	36.955	1.00	74.83	A
ATOM	3432	NZ	LYS	A	468	38.920	1.365	36.764	1.00	74.83	A
ATOM	3433	C	LYS	A	468	37.850	7.492	36.037	1.00	42.40	A
ATOM	3434	O	LYS	A	468	38.295	7.088	34.962	1.00	42.40	A
ATOM	3435	N	GLY	A	469	38.113	8.700	36.521	1.00	46.88	A
ATOM	3436	CA	GLY	A	469	38.981	9.600	35.785	1.00	46.88	A
ATOM	3437	C	GLY	A	469	38.279	10.279	34.625	1.00	46.88	A
ATOM	3438	O	GLY	A	469	38.910	10.997	33.844	1.00	46.88	A
ATOM	3439	N	LYS	A	470	36.970	10.056	34.512	1.00	47.53	A
ATOM	3440	CA	LYS	A	470	36.179	10.650	33.440	1.00	47.53	A
ATOM	3441	CB	LYS	A	470	35.383	9.574	32.704	1.00	66.54	A
ATOM	3442	CG	LYS	A	470	36.119	8.980	31.516	1.00	66.54	A
ATOM	3443	CD	LYS	A	470	37.494	8.481	31.894	1.00	66.54	A
ATOM	3444	CE	LYS	A	470	38.190	7.822	30.710	1.00	66.54	A
ATOM	3445	NZ	LYS	A	470	37.472	6.586	30.287	1.00	66.54	A
ATOM	3446	C	LYS	A	470	35.243	11.716	33.962	1.00	47.53	A
ATOM	3447	O	LYS	A	470	34.720	11.615	35.072	1.00	47.53	A
ATOM	3448	N	GLU	A	471	35.030	12.735	33.141	1.00	48.09	A
ATOM	3449	CA	GLU	A	471	34.180	13.858	33.511	1.00	48.09	A
ATOM	3450	CB	GLU	A	471	34.674	15.128	32.813	1.00	81.57	A
ATOM	3451	CG	GLU	A	471	34.887	16.305	33.748	1.00	81.57	A
ATOM	3452	CD	GLU	A	471	35.385	17.537	33.022	1.00	81.57	A
ATOM	3453	OE1	GLU	A	471	36.456	17.460	32.382	1.00	81.57	A
ATOM	3454	OE2	GLU	A	471	34.706	18.582	33.092	1.00	81.57	A
ATOM	3455	C	GLU	A	471	32.705	13.655	33.186	1.00	48.09	A
ATOM	3456	O	GLU	A	471	31.835	14.164	33.895	1.00	48.09	A
ATOM	3457	N	LEU	A	472	32.413	12.898	32.131	1.00	39.18	A
ATOM	3458	CA	LEU	A	472	31.020	12.718	31.748	1.00	39.18	A

FIGURE 25 CON'T

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ATOM   3459  CB  LEU A 472      30.575  13.901  30.880  1.00 52.26      A
ATOM   3460  CG  LEU A 472      29.125  14.391  30.824  1.00 52.26      A
ATOM   3461  CD1 LEU A 472      28.958  15.236  29.562  1.00 52.26      A
ATOM   3462  CD2 LEU A 472      28.152  13.237  30.810  1.00 52.26      A
ATOM   3463  C   LEU A 472      30.811  11.447  30.973  1.00 39.18      A
ATOM   3464  O   LEU A 472      31.648  11.058  30.158  1.00 39.18      A
ATOM   3465  N   GLY A 473      29.673  10.813  31.225  1.00 40.26      A
ATOM   3466  CA  GLY A 473      29.327   9.598  30.518  1.00 40.26      A
ATOM   3467  C   GLY A 473      27.844   9.640  30.185  1.00 40.26      A
ATOM   3468  O   GLY A 473      27.103  10.446  30.750  1.00 40.26      A
ATOM   3469  N   LEU A 474      27.416   8.775  29.273  1.00 42.74      A
ATOM   3470  CA  LEU A 474      26.017   8.697  28.872  1.00 42.74      A
ATOM   3471  CB  LEU A 474      25.831   9.263  27.458  1.00 61.12      A
ATOM   3472  CG  LEU A 474      25.916  10.784  27.322  1.00 61.12      A
ATOM   3473  CD1 LEU A 474      25.957  11.169  25.855  1.00 61.12      A
ATOM   3474  CD2 LEU A 474      24.718  11.418  28.004  1.00 61.12      A
ATOM   3475  C   LEU A 474      25.566   7.244  28.902  1.00 42.74      A
ATOM   3476  O   LEU A 474      26.281   6.349  28.442  1.00 42.74      A
ATOM   3477  N   ALA A 475      24.388   7.008  29.458  1.00 39.49      A
ATOM   3478  CA  ALA A 475      23.863   5.657  29.523  1.00 39.49      A
ATOM   3479  CB  ALA A 475      23.805   5.168  30.976  1.00 27.45      A
ATOM   3480  C   ALA A 475      22.475   5.601  28.895  1.00 39.49      A
ATOM   3481  O   ALA A 475      21.597   6.398  29.229  1.00 39.49      A
ATOM   3482  N   PHE A 476      22.305   4.657  27.975  1.00 36.70      A
ATOM   3483  CA  PHE A 476      21.040   4.435  27.289  1.00 36.70      A

ATOM   3484  CB  PHE A 476      21.268   4.420  25.776  1.00 42.67      A
ATOM   3485  CG  PHE A 476      21.771   5.732  25.254  1.00 42.67      A
ATOM   3486  CD1 PHE A 476      20.898   6.789  25.044  1.00 42.67      A
ATOM   3487  CD2 PHE A 476      23.132   5.951  25.094  1.00 42.67      A
ATOM   3488  CE1 PHE A 476      21.370   8.051  24.690  1.00 42.67      A
ATOM   3489  CE2 PHE A 476      23.620   7.213  24.740  1.00 42.67      A
ATOM   3490  CZ  PHE A 476      22.735   8.267  24.539  1.00 42.67      A
ATOM   3491  C   PHE A 476      20.562   3.103  27.823  1.00 36.70      A
ATOM   3492  O   PHE A 476      21.233   2.073  27.674  1.00 36.70      A
ATOM   3493  N   ILE A 477      19.396   3.155  28.460  1.00 35.04      A
ATOM   3494  CA  ILE A 477      18.801   2.015  29.122  1.00 35.04      A
ATOM   3495  CB  ILE A 477      18.587   2.373  30.607  1.00 32.38      A
ATOM   3496  CG2 ILE A 477      18.258   1.118  31.410  1.00 32.38      A
ATOM   3497  CG1 ILE A 477      19.854   3.050  31.150  1.00 32.38      A
ATOM   3498  CD1 ILE A 477      19.719   3.619  32.567  1.00 32.38      A
ATOM   3499  C   ILE A 477      17.480   1.494  28.554  1.00 35.04      A
ATOM   3500  O   ILE A 477      16.520   2.241  28.385  1.00 35.04      A
ATOM   3501  N   ALA A 478      17.444   0.198  28.277  1.00 43.08      A
ATOM   3502  CA  ALA A 478      16.246  -0.453  27.769  1.00 43.08      A
ATOM   3503  CB  ALA A 478      16.585  -1.317  26.549  1.00 35.21      A
ATOM   3504  C   ALA A 478      15.786  -1.327  28.922  1.00 43.08      A
ATOM   3505  O   ALA A 478      16.532  -2.199  29.366  1.00 43.08      A
ATOM   3506  N   ALA A 479      14.569  -1.096  29.402  1.00 41.88      A
ATOM   3507  CA  ALA A 479      14.026  -1.856  30.524  1.00 41.88      A
ATOM   3508  CB  ALA A 479      14.095  -1.018  31.773  1.00 31.33      A
ATOM   3509  C   ALA A 479      12.586  -2.314  30.324  1.00 41.88      A
ATOM   3510  O   ALA A 479      11.834  -1.715  29.560  1.00 41.88      A
ATOM   3511  N   ARG A 480      12.202  -3.363  31.043  1.00 51.72      A
ATOM   3512  CA  ARG A 480      10.835  -3.865  30.976  1.00 51.72      A
ATOM   3513  CB  ARG A 480      10.717  -5.184  31.737  1.00 64.52      A
ATOM   3514  CG  ARG A 480      11.683  -6.237  31.248  1.00 64.52      A
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ATOM   3515  CD  ARG A 480      11.326  -7.615  31.746  1.00 64.52      A
ATOM   3516  NE  ARG A 480      11.570  -7.801  33.172  1.00 64.52      A
ATOM   3517  CZ  ARG A 480      12.774  -7.806  33.730  1.00 64.52      A
ATOM   3518  NH1 ARG A 480      13.846  -7.624  32.986  1.00 64.52      A
ATOM   3519  NH2 ARG A 480      12.910  -8.029  35.024  1.00 64.52      A
ATOM   3520  C   ARG A 480       9.943  -2.811  31.625  1.00 51.72      A
ATOM   3521  O   ARG A 480      10.426  -1.972  32.389  1.00 51.72      A
ATOM   3522  N   ASN A 481       8.651  -2.842  31.325  1.00 50.98      A
ATOM   3523  CA  ASN A 481       7.732  -1.867  31.907  1.00 50.98      A
ATOM   3524  CB  ASN A 481       6.393  -1.873  31.165  1.00 75.37      A
ATOM   3525  CG  ASN A 481       6.545  -1.619  29.679  1.00 75.37      A
ATOM   3526  OD1 ASN A 481       7.153  -0.634  29.259  1.00 75.37      A
ATOM   3527  ND2 ASN A 481       5.981  -2.512  28.870  1.00 75.37      A
ATOM   3528  C   ASN A 481       7.482  -2.164  33.386  1.00 50.98      A
ATOM   3529  O   ASN A 481       7.078  -1.281  34.143  1.00 50.98      A
ATOM   3530  N   LYS A 482       7.751  -3.406  33.779  1.00 55.90      A
ATOM   3531  CA  LYS A 482       7.535  -3.894  35.142  1.00 55.90      A
ATOM   3532  CB  LYS A 482       7.775  -5.405  35.193  1.00153.22      A
ATOM   3533  CG  LYS A 482       6.810  -6.238  34.371  1.00153.22      A
ATOM   3534  CD  LYS A 482       7.054  -7.720  34.608  1.00153.22      A
ATOM   3535  CE  LYS A 482       6.021  -8.578  33.901  1.00153.22      A
ATOM   3536  NZ  LYS A 482       6.200 -10.023  34.213  1.00153.22      A
ATOM   3537  C   LYS A 482       8.332  -3.256  36.275  1.00 55.90      A
ATOM   3538  O   LYS A 482       7.918  -3.332  37.434  1.00 55.90      A
ATOM   3539  N   LEU A 483       9.481  -2.661  35.967  1.00 55.02      A
ATOM   3540  CA  LEU A 483      10.291  -2.043  37.013  1.00 55.02      A
ATOM   3541  CB  LEU A 483      11.551  -1.398  36.431  1.00 65.69      A
ATOM   3542  CG  LEU A 483      12.749  -2.294  36.121  1.00 65.69      A
ATOM   3543  CD1 LEU A 483      12.423  -3.201  34.947  1.00 65.69      A
ATOM   3544  CD2 LEU A 483      13.961  -1.421  35.805  1.00 65.69      A
ATOM   3545  C   LEU A 483       9.509  -0.989  37.779  1.00 55.02      A
ATOM   3546  O   LEU A 483       8.807  -0.169  37.186  1.00 55.02      A
ATOM   3547  N   SER A 484       9.635  -1.019  39.101  1.00 57.55      A
ATOM   3548  CA  SER A 484       8.954  -0.052  39.950  1.00 57.55      A
ATOM   3549  CB  SER A 484       9.173  -0.407  41.419  1.00 65.93      A
ATOM   3550  OG  SER A 484      10.555  -0.417  41.727  1.00 65.93      A
ATOM   3551  C   SER A 484       9.543   1.324  39.663  1.00 57.55      A
ATOM   3552  O   SER A 484      10.613   1.422  39.060  1.00 57.55      A
ATOM   3553  N   SER A 485       8.851   2.382  40.078  1.00 68.39      A
ATOM   3554  CA  SER A 485       9.351   3.737  39.856  1.00 68.39      A
ATOM   3555  CB  SER A 485       8.346   4.778  40.350  1.00 92.91      A
ATOM   3556  OG  SER A 485       7.168   4.761  39.569  1.00 92.91      A
ATOM   3557  C   SER A 485      10.650   3.891  40.631  1.00 68.39      A
ATOM   3558  O   SER A 485      11.587   4.552  40.186  1.00 68.39      A
ATOM   3559  N   GLU A 486      10.687   3.253  41.793  1.00 63.66      A
ATOM   3560  CA  GLU A 486      11.837   3.291  42.682  1.00 63.66      A
ATOM   3561  CB  GLU A 486      11.517   2.491  43.946  1.00137.76      A
ATOM   3562  CG  GLU A 486      12.596   2.505  45.006  1.00137.76      A
ATOM   3563  CD  GLU A 486      12.133   1.850  46.291  1.00137.76      A
ATOM   3564  OE1 GLU A 486      11.719   0.672  46.243  1.00137.76      A
ATOM   3565  OE2 GLU A 486      12.180   2.514  47.347  1.00137.76      A
ATOM   3566  C   GLU A 486      13.102   2.753  42.023  1.00 63.66      A
ATOM   3567  O   GLU A 486      14.154   3.394  42.074  1.00 63.66      A
ATOM   3568  N   LYS A 487      13.002   1.578  41.407  1.00 56.40      A
ATOM   3569  CA  LYS A 487      14.156   0.969  40.751  1.00 56.40      A
ATOM   3570  CB  LYS A 487      13.819  -0.451  40.297  1.00 87.04      A
ATOM   3571  CG  LYS A 487      13.731  -1.417  41.465  1.00 87.04      A
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ATOM   3572  CD  LYS A 487      13.418  -2.834  41.032  1.00 87.04      A
ATOM   3573  CE  LYS A 487      13.405  -3.758  42.238  1.00 87.04      A
ATOM   3574  NZ  LYS A 487      12.976  -5.133  41.883  1.00 87.04      A
ATOM   3575  C   LYS A 487      14.679   1.800  39.584  1.00 56.40      A
ATOM   3576  O   LYS A 487      15.885   1.867  39.361  1.00 56.40      A
ATOM   3577  N   PHE A 488      13.777   2.432  38.842  1.00 49.04      A
ATOM   3578  CA  PHE A 488      14.195   3.272  37.736  1.00 49.04      A
ATOM   3579  CB  PHE A 488      12.982   3.769  36.947  1.00 62.57      A
ATOM   3580  CG  PHE A 488      12.550   2.843  35.842  1.00 62.57      A
ATOM   3581  CD1 PHE A 488      13.434   2.494  34.824  1.00 62.57      A
ATOM   3582  CD2 PHE A 488      11.249   2.341  35.801  1.00 62.57      A
ATOM   3583  CE1 PHE A 488      13.030   1.662  33.780  1.00 62.57      A
ATOM   3584  CE2 PHE A 488      10.834   1.506  34.760  1.00 62.57      A
ATOM   3585  CZ  PHE A 488      11.727   1.167  33.747  1.00 62.57      A
ATOM   3586  C   PHE A 488      14.964   4.463  38.326  1.00 49.04      A
ATOM   3587  O   PHE A 488      16.072   4.781  37.882  1.00 49.04      A
ATOM   3588  N   GLU A 489      14.370   5.101  39.337  1.00 55.24      A
ATOM   3589  CA  GLU A 489      14.980   6.248  40.001  1.00 55.24      A
ATOM   3590  CB  GLU A 489      14.055   6.774  41.107  1.00 68.39      A
ATOM   3591  CG  GLU A 489      14.609   7.969  41.883  1.00 68.39      A
ATOM   3592  CD  GLU A 489      14.405   9.298  41.169  1.00 68.39      A
ATOM   3593  OE1 GLU A 489      14.203   9.291  39.935  1.00 68.39      A
ATOM   3594  OE2 GLU A 489      14.458  10.351  41.845  1.00 68.39      A
ATOM   3595  C   GLU A 489      16.342   5.866  40.595  1.00 55.24      A
ATOM   3596  O   GLU A 489      17.320   6.597  40.440  1.00 55.24      A
ATOM   3597  N   GLU A 490      16.410   4.719  41.265  1.00 43.99      A
ATOM   3598  CA  GLU A 490      17.669   4.270  41.866  1.00 43.99      A
ATOM   3599  CB  GLU A 490      17.453   2.968  42.642  1.00158.89      A
ATOM   3600  CG  GLU A 490      16.534   3.124  43.846  1.00158.89      A
ATOM   3601  CD  GLU A 490      16.395   1.844  44.650  1.00158.89      A
ATOM   3602  OE1 GLU A 490      15.979   0.817  44.073  1.00158.89      A
ATOM   3603  OE2 GLU A 490      16.698   1.867  45.861  1.00158.89      A
ATOM   3604  C   GLU A 490      18.766   4.084  40.816  1.00 43.99      A
ATOM   3605  O   GLU A 490      19.922   4.490  41.015  1.00 43.99      A
ATOM   3606  N   ILE A 491      18.402   3.473  39.691  1.00 40.00      A
ATOM   3607  CA  ILE A 491      19.357   3.254  38.607  1.00 40.00      A
ATOM   3608  CB  ILE A 491      18.687   2.515  37.418  1.00 42.91      A
ATOM   3609  CG2 ILE A 491      19.604   2.542  36.188  1.00 42.91      A
ATOM   3610  CG1 ILE A 491      18.362   1.070  37.823  1.00 42.91      A
ATOM   3611  CD1 ILE A 491      17.546   0.328  36.790  1.00 42.91      A

ATOM   3612  C   ILE A 491      19.923   4.585  38.114  1.00 40.00      A
ATOM   3613  O   ILE A 491      21.137   4.754  38.016  1.00 40.00      A
ATOM   3614  N   LYS A 492      19.034   5.530  37.825  1.00 45.61      A
ATOM   3615  CA  LYS A 492      19.434   6.838  37.322  1.00 45.61      A
ATOM   3616  CB  LYS A 492      18.200   7.647  36.911  1.00 73.74      A
ATOM   3617  CG  LYS A 492      17.380   7.014  35.795  1.00 73.74      A
ATOM   3618  CD  LYS A 492      16.412   8.012  35.170  1.00 73.74      A
ATOM   3619  CE  LYS A 492      15.412   8.545  36.182  1.00 73.74      A
ATOM   3620  NZ  LYS A 492      14.528   9.595  35.592  1.00 73.74      A
ATOM   3621  C   LYS A 492      20.273   7.662  38.300  1.00 45.61      A
ATOM   3622  O   LYS A 492      21.271   8.277  37.902  1.00 45.61      A
ATOM   3623  N   ARG A 493      19.863   7.675  39.569  1.00 38.59      A
ATOM   3624  CA  ARG A 493      20.562   8.436  40.594  1.00 38.59      A
ATOM   3625  CB  ARG A 493      19.751   8.412  41.905  1.00 58.59      A
ATOM   3626  CG  ARG A 493      20.469   9.034  43.107  1.00 58.59      A
ATOM   3627  CD  ARG A 493      19.544   9.274  44.297  1.00 58.59      A
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FIGURE 25 CON'T
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ATOM   3628  NE  ARG A 493      18.748   8.099  44.628  1.00 58.59      A
ATOM   3629  CZ  ARG A 493      19.232   6.981  45.159  1.00 58.59      A
ATOM   3630  NH1 ARG A 493      20.528   6.876  45.441  1.00 58.59      A
ATOM   3631  NH2 ARG A 493      18.415   5.954  45.381  1.00 58.59      A
ATOM   3632  C   ARG A 493      21.982   7.899  40.818  1.00 38.59      A
ATOM   3633  O   ARG A 493      22.944   8.672  40.889  1.00 38.59      A
ATOM   3634  N   ARG A 494      22.109   6.580  40.910  1.00 44.47      A
ATOM   3635  CA  ARG A 494      23.413   5.946  41.125  1.00 44.47      A
ATOM   3636  CB  ARG A 494      23.241   4.450  41.398  1.00 70.57      A
ATOM   3637  CG  ARG A 494      22.684   4.145  42.775  1.00 70.57      A
ATOM   3638  CD  ARG A 494      22.649   2.651  43.029  1.00 70.57      A
ATOM   3639  NE  ARG A 494      22.421   2.341  44.435  1.00 70.57      A
ATOM   3640  CZ  ARG A 494      21.321   2.662  45.110  1.00 70.57      A
ATOM   3641  NH1 ARG A 494      20.327   3.313  44.513  1.00 70.57      A
ATOM   3642  NH2 ARG A 494      21.216   2.328  46.389  1.00 70.57      A
ATOM   3643  C   ARG A 494      24.359   6.146  39.943  1.00 44.47      A
ATOM   3644  O   ARG A 494      25.572   6.294  40.129  1.00 44.47      A
ATOM   3645  N   LEU A 495      23.820   6.142  38.726  1.00 32.24      A
ATOM   3646  CA  LEU A 495      24.685   6.358  37.578  1.00 32.24      A
ATOM   3647  CB  LEU A 495      23.971   6.042  36.266  1.00 37.98      A
ATOM   3648  CG  LEU A 495      23.668   4.549  36.102  1.00 37.98      A
ATOM   3649  CD1 LEU A 495      22.747   4.315  34.894  1.00 37.98      A
ATOM   3650  CD2 LEU A 495      24.977   3.784  35.968  1.00 37.98      A
ATOM   3651  C   LEU A 495      25.132   7.800  37.598  1.00 32.24      A
ATOM   3652  O   LEU A 495      26.296   8.098  37.290  1.00 32.24      A
ATOM   3653  N   PHE A 496      24.238   8.704  37.992  1.00 41.94      A
ATOM   3654  CA  PHE A 496      24.641  10.097  38.011  1.00 41.94      A
ATOM   3655  CB  PHE A 496      23.471  11.053  38.247  1.00 34.82      A
ATOM   3656  CG  PHE A 496      23.860  12.502  38.070  1.00 34.82      A
ATOM   3657  CD1 PHE A 496      24.164  13.001  36.806  1.00 34.82      A
ATOM   3658  CD2 PHE A 496      24.033  13.330  39.169  1.00 34.82      A
ATOM   3659  CE1 PHE A 496      24.646  14.303  36.641  1.00 34.82      A
ATOM   3660  CE2 PHE A 496      24.516  14.636  39.021  1.00 34.82      A
ATOM   3661  CZ  PHE A 496      24.825  15.124  37.752  1.00 34.82      A
ATOM   3662  C   PHE A 496      25.723  10.373  39.051  1.00 41.94      A
ATOM   3663  O   PHE A 496      26.532  11.277  38.860  1.00 41.94      A
ATOM   3664  N   ASN A 497      25.737   9.624  40.153  1.00 43.40      A
ATOM   3665  CA  ASN A 497      26.779   9.837  41.160  1.00 43.40      A
ATOM   3666  CB  ASN A 497      26.649   8.862  42.334  1.00 48.67      A
ATOM   3667  CG  ASN A 497      25.547   9.250  43.293  1.00 48.67      A
ATOM   3668  OD1 ASN A 497      25.153  10.415  43.361  1.00 48.67      A
ATOM   3669  ND2 ASN A 497      25.050   8.279  44.053  1.00 48.67      A
ATOM   3670  C   ASN A 497      28.117   9.617  40.476  1.00 43.40      A
ATOM   3671  O   ASN A 497      29.145  10.132  40.914  1.00 43.40      A
ATOM   3672  N   LEU A 498      28.083   8.864  39.380  1.00 44.31      A
ATOM   3673  CA  LEU A 498      29.283   8.562  38.610  1.00 44.31      A
ATOM   3674  CB  LEU A 498      29.213   7.125  38.102  1.00 39.12      A
ATOM   3675  CG  LEU A 498      28.996   6.073  39.187  1.00 39.12      A
ATOM   3676  CD1 LEU A 498      28.786   4.711  38.542  1.00 39.12      A
ATOM   3677  CD2 LEU A 498      30.208   6.052  40.119  1.00 39.12      A
ATOM   3678  C   LEU A 498      29.485   9.502  37.421  1.00 44.31      A
ATOM   3679  O   LEU A 498      30.307   9.230  36.547  1.00 44.31      A
ATOM   3680  N   ASN A 499      28.751  10.610  37.394  1.00 41.29      A
ATOM   3681  CA  ASN A 499      28.840  11.562  36.281  1.00 41.29      A
ATOM   3682  CB  ASN A 499      30.289  11.976  35.981  1.00 51.72      A
ATOM   3683  CG  ASN A 499      30.914  12.799  37.082  1.00 51.72      A
ATOM   3684  OD1 ASN A 499      30.276  13.670  37.672  1.00 51.72      A
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FIGURE 25 CON'T

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ATOM   3685  ND2 ASN A 499      32.191  12.540  37.346  1.00 51.72      A
ATOM   3686  C   ASN A 499      28.264  10.967  35.000  1.00 41.29      A
ATOM   3687  O   ASN A 499      28.703  11.312  33.902  1.00 41.29      A
ATOM   3688  N   VAL A 500      27.303  10.062  35.131  1.00 42.36      A
ATOM   3689  CA  VAL A 500      26.696   9.463  33.952  1.00 42.36      A
ATOM   3690  CB  VAL A 500      26.783   7.916  34.003  1.00 38.46      A
ATOM   3691  CG1 VAL A 500      26.070   7.305  32.786  1.00 38.46      A
ATOM   3692  CG2 VAL A 500      28.259   7.483  34.017  1.00 38.46      A
ATOM   3693  C   VAL A 500      25.238   9.891  33.848  1.00 42.36      A
ATOM   3694  O   VAL A 500      24.434   9.628  34.753  1.00 42.36      A
ATOM   3695  N   ILE A 501      24.909  10.572  32.755  1.00 36.97      A
ATOM   3696  CA  ILE A 501      23.545  11.027  32.521  1.00 36.97      A
ATOM   3697  CB  ILE A 501      23.498  12.270  31.587  1.00 40.00      A
ATOM   3698  CG2 ILE A 501      22.047  12.747  31.416  1.00 40.00      A
ATOM   3699  CG1 ILE A 501      24.383  13.393  32.140  1.00 40.00      A
ATOM   3700  CD1 ILE A 501      24.030  13.826  33.503  1.00 40.00      A
ATOM   3701  C   ILE A 501      22.888   9.855  31.803  1.00 36.97      A
ATOM   3702  O   ILE A 501      23.525   9.217  30.965  1.00 36.97      A
ATOM   3703  N   SER A 502      21.632   9.563  32.113  1.00 35.35      A
ATOM   3704  CA  SER A 502      20.978   8.435  31.463  1.00 35.35      A
ATOM   3705  CB  SER A 502      20.817   7.293  32.465  1.00 45.93      A
ATOM   3706  OG  SER A 502      20.206   7.765  33.644  1.00 45.93      A
ATOM   3707  C   SER A 502      19.630   8.732  30.796  1.00 35.35      A
ATOM   3708  O   SER A 502      18.951   9.706  31.115  1.00 35.35      A
ATOM   3709  N   GLN A 503      19.257   7.866  29.862  1.00 37.71      A
ATOM   3710  CA  GLN A 503      18.008   8.006  29.124  1.00 37.71      A
ATOM   3711  CB  GLN A 503      18.284   8.537  27.709  1.00 48.11      A
ATOM   3712  CG  GLN A 503      17.046   8.679  26.840  1.00 48.11      A
ATOM   3713  CD  GLN A 503      16.065   9.680  27.410  1.00 48.11      A
ATOM   3714  OE1 GLN A 503      16.450  10.786  27.792  1.00 48.11      A
ATOM   3715  NE2 GLN A 503      14.790   9.302  27.469  1.00 48.11      A
ATOM   3716  C   GLN A 503      17.381   6.616  29.042  1.00 37.71      A
ATOM   3717  O   GLN A 503      17.978   5.680  28.494  1.00 37.71      A
ATOM   3718  N   VAL A 504      16.182   6.493  29.587  1.00 44.85      A
ATOM   3719  CA  VAL A 504      15.480   5.225  29.600  1.00 44.85      A
ATOM   3720  CB  VAL A 504      14.784   4.983  30.960  1.00 45.98      A
ATOM   3721  CG1 VAL A 504      14.143   3.604  30.968  1.00 45.98      A
ATOM   3722  CG2 VAL A 504      15.777   5.126  32.099  1.00 45.98      A
ATOM   3723  C   VAL A 504      14.400   5.124  28.536  1.00 44.85      A
ATOM   3724  O   VAL A 504      13.630   6.056  28.332  1.00 44.85      A
ATOM   3725  N   VAL A 505      14.360   3.983  27.861  1.00 43.58      A
ATOM   3726  CA  VAL A 505      13.337   3.685  26.866  1.00 43.58      A
ATOM   3727  CB  VAL A 505      13.942   3.523  25.458  1.00 38.53      A
ATOM   3728  CG1 VAL A 505      12.844   3.259  24.454  1.00 38.53      A
ATOM   3729  CG2 VAL A 505      14.695   4.777  25.068  1.00 38.53      A
ATOM   3730  C   VAL A 505      12.761   2.349  27.355  1.00 43.58      A
ATOM   3731  O   VAL A 505      13.493   1.363  27.490  1.00 43.58      A
ATOM   3732  N   ASN A 506      11.468   2.318  27.664  1.00 46.42      A
ATOM   3733  CA  ASN A 506      10.859   1.085  28.159  1.00 46.42      A
ATOM   3734  CB  ASN A 506       9.706   1.386  29.129  1.00 59.81      A
ATOM   3735  CG  ASN A 506       8.601   2.214  28.493  1.00 59.81      A
ATOM   3736  OD1 ASN A 506       8.264   2.030  27.326  1.00 59.81      A
ATOM   3737  ND2 ASN A 506       8.022   3.122  29.269  1.00 59.81      A
ATOM   3738  C   ASN A 506      10.363   0.172  27.048  1.00 46.42      A
ATOM   3739  O   ASN A 506      10.230   0.587  25.902  1.00 46.42      A

ATOM   3740  N   GLU A 507      10.095  -1.077  27.404  1.00 50.99      A
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FIGURE 25 CON'T

ATOM	3741	CA	GLU	A	507	9.627	-2.074	26.453	1.00	50.99	A
ATOM	3742	CB	GLU	A	507	9.361	-3.395	27.181	1.00	59.87	A
ATOM	3743	CG	GLU	A	507	9.132	-4.572	26.245	1.00	59.87	A
ATOM	3744	CD	GLU	A	507	9.013	-5.901	26.970	1.00	59.87	A
ATOM	3745	OE1	GLU	A	507	9.278	-6.942	26.325	1.00	59.87	A
ATOM	3746	OE2	GLU	A	507	8.648	-5.912	28.172	1.00	59.87	A
ATOM	3747	C	GLU	A	507	8.376	-1.659	25.653	1.00	50.99	A
ATOM	3748	O	GLU	A	507	8.222	-2.060	24.491	1.00	50.99	A
ATOM	3749	N	ASP	A	508	7.491	-0.865	26.253	1.00	52.41	A
ATOM	3750	CA	ASP	A	508	6.282	-0.443	25.544	1.00	52.41	A
ATOM	3751	CB	ASP	A	508	5.348	0.355	26.457	1.00	74.58	A
ATOM	3752	CG	ASP	A	508	4.045	0.739	25.760	1.00	74.58	A
ATOM	3753	OD1	ASP	A	508	3.995	1.799	25.097	1.00	74.58	A
ATOM	3754	OD2	ASP	A	508	3.069	-0.035	25.860	1.00	74.58	A
ATOM	3755	C	ASP	A	508	6.618	0.392	24.314	1.00	52.41	A
ATOM	3756	O	ASP	A	508	6.090	0.154	23.225	1.00	52.41	A
ATOM	3757	N	THR	A	509	7.494	1.370	24.491	1.00	49.23	A
ATOM	3758	CA	THR	A	509	7.898	2.218	23.390	1.00	49.23	A
ATOM	3759	CB	THR	A	509	8.894	3.294	23.860	1.00	43.42	A
ATOM	3760	OG1	THR	A	509	8.289	4.091	24.884	1.00	43.42	A
ATOM	3761	CG2	THR	A	509	9.296	4.171	22.703	1.00	43.42	A
ATOM	3762	C	THR	A	509	8.571	1.383	22.304	1.00	49.23	A
ATOM	3763	O	THR	A	509	8.295	1.552	21.121	1.00	49.23	A
ATOM	3764	N	LEU	A	510	9.448	0.476	22.719	1.00	56.19	A
ATOM	3765	CA	LEU	A	510	10.172	-0.370	21.787	1.00	56.19	A
ATOM	3766	CB	LEU	A	510	11.199	-1.220	22.539	1.00	52.24	A
ATOM	3767	CG	LEU	A	510	12.326	-0.427	23.220	1.00	52.24	A
ATOM	3768	CD1	LEU	A	510	13.142	-1.331	24.147	1.00	52.24	A
ATOM	3769	CD2	LEU	A	510	13.210	0.201	22.150	1.00	52.24	A
ATOM	3770	C	LEU	A	510	9.268	-1.264	20.949	1.00	56.19	A
ATOM	3771	O	LEU	A	510	9.521	-1.459	19.758	1.00	56.19	A
ATOM	3772	N	LYS	A	511	8.209	-1.798	21.548	1.00	51.64	A
ATOM	3773	CA	LYS	A	511	7.313	-2.670	20.795	1.00	51.64	A
ATOM	3774	CB	LYS	A	511	6.653	-3.703	21.713	1.00	94.73	A
ATOM	3775	CG	LYS	A	511	7.585	-4.810	22.183	1.00	94.73	A
ATOM	3776	CD	LYS	A	511	6.809	-6.037	22.643	1.00	94.73	A
ATOM	3777	CE	LYS	A	511	5.841	-5.711	23.769	1.00	94.73	A
ATOM	3778	NZ	LYS	A	511	5.049	-6.906	24.160	1.00	94.73	A
ATOM	3779	C	LYS	A	511	6.221	-1.965	19.997	1.00	51.64	A
ATOM	3780	O	LYS	A	511	5.881	-2.411	18.901	1.00	51.64	A
ATOM	3781	N	ASN	A	512	5.702	-0.854	20.516	1.00	57.85	A
ATOM	3782	CA	ASN	A	512	4.600	-0.154	19.857	1.00	57.85	A
ATOM	3783	CB	ASN	A	512	3.480	0.069	20.873	1.00	59.41	A
ATOM	3784	CG	ASN	A	512	3.127	-1.192	21.621	1.00	59.41	A
ATOM	3785	OD1	ASN	A	512	2.917	-2.241	21.017	1.00	59.41	A
ATOM	3786	ND2	ASN	A	512	3.063	-1.100	22.943	1.00	59.41	A
ATOM	3787	C	ASN	A	512	4.845	1.164	19.129	1.00	57.85	A
ATOM	3788	O	ASN	A	512	3.890	1.782	18.665	1.00	57.85	A
ATOM	3789	N	LYS	A	513	6.092	1.610	19.021	1.00	49.76	A
ATOM	3790	CA	LYS	A	513	6.345	2.876	18.341	1.00	49.76	A
ATOM	3791	CB	LYS	A	513	6.929	3.884	19.330	1.00	70.06	A
ATOM	3792	CG	LYS	A	513	6.139	4.014	20.631	1.00	70.06	A
ATOM	3793	CD	LYS	A	513	4.735	4.560	20.406	1.00	70.06	A
ATOM	3794	CE	LYS	A	513	3.942	4.630	21.715	1.00	70.06	A
ATOM	3795	NZ	LYS	A	513	4.545	5.562	22.721	1.00	70.06	A
ATOM	3796	C	LYS	A	513	7.286	2.706	17.146	1.00	49.76	A
ATOM	3797	O	LYS	A	513	8.074	3.597	16.826	1.00	49.76	A

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ATOM   3798  N   ARG A 514       7.193   1.561  16.481  1.00 51.04      A
ATOM   3799  CA  ARG A 514       8.050   1.279  15.335  1.00 51.04      A
ATOM   3800  CB  ARG A 514       8.111  -0.233  15.098  1.00 95.38      A
ATOM   3801  CG  ARG A 514       8.587  -1.013  16.315  1.00 95.38      A
ATOM   3802  CD  ARG A 514       8.878  -2.471  15.996  1.00 95.38      A
ATOM   3803  NE  ARG A 514       9.496  -3.151  17.133  1.00 95.38      A
ATOM   3804  CZ  ARG A 514      10.039  -4.364  17.083  1.00 95.38      A
ATOM   3805  NH1 ARG A 514      10.046  -5.044  15.945  1.00 95.38      A
ATOM   3806  NH2 ARG A 514      10.582  -4.897  18.172  1.00 95.38      A
ATOM   3807  C   ARG A 514       7.599   1.994  14.059  1.00 51.04      A
ATOM   3808  O   ARG A 514       6.404   2.179  13.822  1.00 51.04      A
ATOM   3809  N   ASP A 515       8.565   2.406  13.241  1.00 46.95      A
ATOM   3810  CA  ASP A 515       8.252   3.090  11.987  1.00 46.95      A
ATOM   3811  CB  ASP A 515       9.536   3.522  11.279  1.00 87.61      A
ATOM   3812  CG  ASP A 515       9.282   4.543  10.191  1.00 87.61      A
ATOM   3813  OD1 ASP A 515       8.817   5.657  10.519  1.00 87.61      A
ATOM   3814  OD2 ASP A 515       9.541   4.233   9.012  1.00 87.61      A
ATOM   3815  C   ASP A 515       7.458   2.128  11.091  1.00 46.95      A
ATOM   3816  O   ASP A 515       7.786   0.944  10.992  1.00 46.95      A
ATOM   3817  N   LYS A 516       6.413   2.639  10.451  1.00 56.69      A
ATOM   3818  CA  LYS A 516       5.572   1.814   9.582  1.00 56.69      A
ATOM   3819  CB  LYS A 516       4.366   2.619   9.087  1.00133.08      A
ATOM   3820  CG  LYS A 516       3.336   2.925  10.162  1.00133.08      A
ATOM   3821  CD  LYS A 516       2.118   3.617   9.568  1.00133.08      A
ATOM   3822  CE  LYS A 516       1.061   3.889  10.625  1.00133.08      A
ATOM   3823  NZ  LYS A 516      -0.126   4.578  10.045  1.00133.08      A
ATOM   3824  C   LYS A 516       6.303   1.221   8.379  1.00 56.69      A
ATOM   3825  O   LYS A 516       5.943   0.147   7.899  1.00 56.69      A
ATOM   3826  N   TYR A 517       7.330   1.910   7.899  1.00 62.90      A
ATOM   3827  CA  TYR A 517       8.072   1.428   6.742  1.00 62.90      A
ATOM   3828  CB  TYR A 517       8.406   2.610   5.824  1.00 60.86      A
ATOM   3829  CG  TYR A 517       7.175   3.178   5.154  1.00 60.86      A
ATOM   3830  CD1 TYR A 517       6.535   2.478   4.135  1.00 60.86      A
ATOM   3831  CE1 TYR A 517       5.360   2.957   3.556  1.00 60.86      A
ATOM   3832  CD2 TYR A 517       6.613   4.383   5.583  1.00 60.86      A
ATOM   3833  CE2 TYR A 517       5.435   4.871   5.015  1.00 60.86      A
ATOM   3834  CZ  TYR A 517       4.815   4.149   4.003  1.00 60.86      A
ATOM   3835  OH  TYR A 517       3.644   4.601   3.450  1.00 60.86      A
ATOM   3836  C   TYR A 517       9.333   0.634   7.077  1.00 62.90      A
ATOM   3837  O   TYR A 517      10.028   0.157   6.179  1.00 62.90      A
ATOM   3838  N   ASP A 518       9.618   0.478   8.366  1.00 51.19      A
ATOM   3839  CA  ASP A 518      10.798  -0.268   8.798  1.00 51.19      A
ATOM   3840  CB  ASP A 518      12.052   0.601   8.635  1.00 47.24      A
ATOM   3841  CG  ASP A 518      13.313  -0.100   9.112  1.00 47.24      A
ATOM   3842  OD1 ASP A 518      13.266  -1.324   9.357  1.00 47.24      A
ATOM   3843  OD2 ASP A 518      14.353   0.571   9.237  1.00 47.24      A
ATOM   3844  C   ASP A 518      10.619  -0.677  10.259  1.00 51.19      A
ATOM   3845  O   ASP A 518      10.949   0.087  11.174  1.00 51.19      A
ATOM   3846  N   ARG A 519      10.092  -1.877  10.476  1.00 59.86      A
ATOM   3847  CA  ARG A 519       9.847  -2.346  11.831  1.00 59.86      A
ATOM   3848  CB  ARG A 519       9.089  -3.673  11.817  1.00124.95      A
ATOM   3849  CG  ARG A 519       9.832  -4.834  11.189  1.00124.95      A
ATOM   3850  CD  ARG A 519       9.214  -6.135  11.662  1.00124.95      A
ATOM   3851  NE  ARG A 519       7.756  -6.046  11.675  1.00124.95      A
ATOM   3852  CZ  ARG A 519       6.957  -6.917  12.283  1.00124.95      A
ATOM   3853  NH1 ARG A 519       7.472  -7.952  12.932  1.00124.95      A
ATOM   3854  NH2 ARG A 519       5.641  -6.747  12.249  1.00124.95      A
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FIGURE 25 CON'T

ATOM	3855	C	ARG	A	519	11.096	-2.497	12.691	1.00	59.86	A
ATOM	3856	O	ARG	A	519	10.992	-2.766	13.883	1.00	59.86	A
ATOM	3857	N	ASN	A	520	12.273	-2.343	12.097	1.00	58.96	A
ATOM	3858	CA	ASN	A	520	13.502	-2.461	12.873	1.00	58.96	A
ATOM	3859	CB	ASN	A	520	14.560	-3.239	12.093	1.00	76.47	A
ATOM	3860	CG	ASN	A	520	14.190	-4.695	11.924	1.00	76.47	A
ATOM	3861	OD1	ASN	A	520	13.951	-5.401	12.903	1.00	76.47	A
ATOM	3862	ND2	ASN	A	520	14.134	-5.153	10.678	1.00	76.47	A
ATOM	3863	C	ASN	A	520	13.996	-1.063	13.195	1.00	58.96	A
ATOM	3864	O	ASN	A	520	15.175	-0.841	13.470	1.00	58.96	A
ATOM	3865	N	ARG	A	521	13.059	-0.127	13.172	1.00	50.69	A
ATOM	3866	CA	ARG	A	521	13.358	1.263	13.436	1.00	50.69	A
ATOM	3867	CB	ARG	A	521	13.494	2.010	12.109	1.00	75.22	A
ATOM	3868	CG	ARG	A	521	13.944	3.443	12.235	1.00	75.22	A
ATOM	3869	CD	ARG	A	521	13.681	4.193	10.950	1.00	75.22	A
ATOM	3870	NE	ARG	A	521	14.171	3.460	9.790	1.00	75.22	A
ATOM	3871	CZ	ARG	A	521	14.201	3.955	8.560	1.00	75.22	A
ATOM	3872	NH1	ARG	A	521	13.769	5.189	8.335	1.00	75.22	A
ATOM	3873	NH2	ARG	A	521	14.662	3.218	7.557	1.00	75.22	A
ATOM	3874	C	ARG	A	521	12.232	1.888	14.265	1.00	50.69	A
ATOM	3875	O	ARG	A	521	11.045	1.589	14.071	1.00	50.69	A
ATOM	3876	N	LEU	A	522	12.616	2.765	15.181	1.00	49.36	A
ATOM	3877	CA	LEU	A	522	11.652	3.438	16.028	1.00	49.36	A
ATOM	3878	CB	LEU	A	522	12.378	4.039	17.232	1.00	57.92	A
ATOM	3879	CG	LEU	A	522	11.813	3.832	18.638	1.00	57.92	A
ATOM	3880	CD1	LEU	A	522	11.188	2.456	18.776	1.00	57.92	A
ATOM	3881	CD2	LEU	A	522	12.942	4.029	19.650	1.00	57.92	A
ATOM	3882	C	LEU	A	522	10.993	4.532	15.197	1.00	49.36	A
ATOM	3883	O	LEU	A	522	11.555	4.983	14.190	1.00	49.36	A
ATOM	3884	N	ASP	A	523	9.796	4.937	15.615	1.00	56.16	A
ATOM	3885	CA	ASP	A	523	9.021	5.985	14.951	1.00	56.16	A
ATOM	3886	CB	ASP	A	523	7.761	6.291	15.764	1.00	97.14	A
ATOM	3887	CG	ASP	A	523	6.495	6.025	14.997	1.00	97.14	A
ATOM	3888	OD1	ASP	A	523	6.320	6.639	13.925	1.00	97.14	A
ATOM	3889	OD2	ASP	A	523	5.675	5.206	15.467	1.00	97.14	A
ATOM	3890	C	ASP	A	523	9.828	7.271	14.834	1.00	56.16	A
ATOM	3891	O	ASP	A	523	10.724	7.521	15.638	1.00	56.16	A
ATOM	3892	N	LEU	A	524	9.487	8.099	13.849	1.00	51.60	A
ATOM	3893	CA	LEU	A	524	10.181	9.365	13.650	1.00	51.60	A
ATOM	3894	CB	LEU	A	524	9.813	9.968	12.290	1.00	64.33	A
ATOM	3895	CG	LEU	A	524	10.572	11.234	11.873	1.00	64.33	A
ATOM	3896	CD1	LEU	A	524	12.066	10.928	11.765	1.00	64.33	A
ATOM	3897	CD2	LEU	A	524	10.046	11.735	10.535	1.00	64.33	A
ATOM	3898	C	LEU	A	524	9.819	10.349	14.766	1.00	51.60	A
ATOM	3899	O	LEU	A	524	10.649	11.144	15.200	1.00	51.60	A
ATOM	3900	N	PHE	A	525	8.572	10.300	15.218	1.00	49.11	A
ATOM	3901	CA	PHE	A	525	8.116	11.186	16.288	1.00	49.11	A
ATOM	3902	CB	PHE	A	525	6.636	10.943	16.580	1.00	60.02	A
ATOM	3903	CG	PHE	A	525	6.102	11.751	17.738	1.00	60.02	A
ATOM	3904	CD1	PHE	A	525	6.015	13.139	17.657	1.00	60.02	A
ATOM	3905	CD2	PHE	A	525	5.665	11.122	18.902	1.00	60.02	A
ATOM	3906	CE1	PHE	A	525	5.496	13.886	18.718	1.00	60.02	A
ATOM	3907	CE2	PHE	A	525	5.146	11.861	19.965	1.00	60.02	A
ATOM	3908	CZ	PHE	A	525	5.060	13.243	19.873	1.00	60.02	A
ATOM	3909	C	PHE	A	525	8.930	10.895	17.548	1.00	49.11	A
ATOM	3910	O	PHE	A	525	9.519	11.786	18.148	1.00	49.11	A

FIGURE 25 CON'T

ATOM	3911	N	VAL	A	526	8.935	9.627	17.939	1.00	45.36	A
ATOM	3912	CA	VAL	A	526	9.656	9.164	19.110	1.00	45.36	A
ATOM	3913	CB	VAL	A	526	9.429	7.648	19.310	1.00	54.70	A
ATOM	3914	CG1	VAL	A	526	10.281	7.125	20.452	1.00	54.70	A
ATOM	3915	CG2	VAL	A	526	7.957	7.388	19.595	1.00	54.70	A
ATOM	3916	C	VAL	A	526	11.151	9.459	18.996	1.00	45.36	A
ATOM	3917	O	VAL	A	526	11.757	9.972	19.936	1.00	45.36	A
ATOM	3918	N	ARG	A	527	11.744	9.154	17.845	1.00	46.49	A
ATOM	3919	CA	ARG	A	527	13.168	9.406	17.665	1.00	46.49	A
ATOM	3920	CB	ARG	A	527	13.619	9.000	16.267	1.00	49.55	A
ATOM	3921	CG	ARG	A	527	13.832	7.501	16.119	1.00	49.55	A
ATOM	3922	CD	ARG	A	527	14.556	7.187	14.826	1.00	49.55	A
ATOM	3923	NE	ARG	A	527	15.108	5.837	14.829	1.00	49.55	A
ATOM	3924	CZ	ARG	A	527	15.989	5.399	13.938	1.00	49.55	A
ATOM	3925	NH1	ARG	A	527	16.406	6.210	12.972	1.00	49.55	A
ATOM	3926	NH2	ARG	A	527	16.471	4.162	14.024	1.00	49.55	A
ATOM	3927	C	ARG	A	527	13.537	10.862	17.933	1.00	46.49	A
ATOM	3928	O	ARG	A	527	14.530	11.137	18.616	1.00	46.49	A
ATOM	3929	N	HIS	A	528	12.748	11.792	17.404	1.00	44.86	A
ATOM	3930	CA	HIS	A	528	13.020	13.209	17.632	1.00	44.86	A
ATOM	3931	CB	HIS	A	528	12.011	14.100	16.897	1.00	54.69	A
ATOM	3932	CG	HIS	A	528	12.390	14.415	15.485	1.00	54.69	A
ATOM	3933	CD2	HIS	A	528	13.002	15.498	14.950	1.00	54.69	A
ATOM	3934	ND1	HIS	A	528	12.142	13.557	14.436	1.00	54.69	A
ATOM	3935	CE1	HIS	A	528	12.580	14.099	13.314	1.00	54.69	A
ATOM	3936	NE2	HIS	A	528	13.107	15.277	13.598	1.00	54.69	A
ATOM	3937	C	HIS	A	528	12.953	13.536	19.121	1.00	44.86	A
ATOM	3938	O	HIS	A	528	13.829	14.216	19.665	1.00	44.86	A
ATOM	3939	N	ASN	A	529	11.904	13.062	19.781	1.00	44.63	A
ATOM	3940	CA	ASN	A	529	11.744	13.348	21.199	1.00	44.63	A
ATOM	3941	CB	ASN	A	529	10.326	12.994	21.632	1.00	60.00	A
ATOM	3942	CG	ASN	A	529	9.300	13.998	21.102	1.00	60.00	A
ATOM	3943	OD1	ASN	A	529	9.293	15.169	21.505	1.00	60.00	A
ATOM	3944	ND2	ASN	A	529	8.445	13.551	20.184	1.00	60.00	A
ATOM	3945	C	ASN	A	529	12.811	12.686	22.079	1.00	44.63	A
ATOM	3946	O	ASN	A	529	13.228	13.266	23.074	1.00	44.63	A
ATOM	3947	N	LEU	A	530	13.273	11.498	21.708	1.00	40.73	A
ATOM	3948	CA	LEU	A	530	14.327	10.854	22.483	1.00	40.73	A
ATOM	3949	CB	LEU	A	530	14.671	9.473	21.920	1.00	47.00	A
ATOM	3950	CG	LEU	A	530	13.791	8.315	22.388	1.00	47.00	A
ATOM	3951	CD1	LEU	A	530	14.301	7.016	21.747	1.00	47.00	A
ATOM	3952	CD2	LEU	A	530	13.820	8.226	23.934	1.00	47.00	A
ATOM	3953	C	LEU	A	530	15.546	11.762	22.399	1.00	40.73	A
ATOM	3954	O	LEU	A	530	16.183	12.050	23.411	1.00	40.73	A
ATOM	3955	N	LEU	A	531	15.849	12.217	21.186	1.00	39.87	A
ATOM	3956	CA	LEU	A	531	16.974	13.111	20.971	1.00	39.87	A
ATOM	3957	CB	LEU	A	531	17.130	13.380	19.470	1.00	52.35	A
ATOM	3958	CG	LEU	A	531	18.335	14.144	18.922	1.00	52.35	A
ATOM	3959	CD1	LEU	A	531	19.639	13.683	19.562	1.00	52.35	A
ATOM	3960	CD2	LEU	A	531	18.382	13.909	17.419	1.00	52.35	A
ATOM	3961	C	LEU	A	531	16.790	14.418	21.754	1.00	39.87	A
ATOM	3962	O	LEU	A	531	17.754	14.931	22.333	1.00	39.87	A
ATOM	3963	N	PHE	A	532	15.563	14.954	21.789	1.00	39.21	A
ATOM	3964	CA	PHE	A	532	15.292	16.197	22.538	1.00	39.21	A
ATOM	3965	CB	PHE	A	532	13.840	16.666	22.367	1.00	45.18	A
ATOM	3966	CG	PHE	A	532	13.475	17.085	20.971	1.00	45.18	A
ATOM	3967	CD1	PHE	A	532	14.452	17.344	20.012	1.00	45.18	A

FIGURE 25 CON'T

ATOM	3968	CD2	PHE	A	532	12.131	17.232	20.619	1.00	45.18	A
ATOM	3969	CE1	PHE	A	532	14.100	17.741	18.717	1.00	45.18	A
ATOM	3970	CE2	PHE	A	532	11.761	17.632	19.318	1.00	45.18	A
ATOM	3971	CZ	PHE	A	532	12.746	17.885	18.369	1.00	45.18	A
ATOM	3972	C	PHE	A	532	15.518	16.000	24.047	1.00	39.21	A
ATOM	3973	O	PHE	A	532	16.051	16.876	24.729	1.00	39.21	A
ATOM	3974	N	GLN	A	533	15.068	14.857	24.562	1.00	36.89	A
ATOM	3975	CA	GLN	A	533	15.202	14.536	25.979	1.00	36.89	A
ATOM	3976	CB	GLN	A	533	14.529	13.202	26.293	1.00	50.19	A
ATOM	3977	CG	GLN	A	533	13.024	13.284	26.378	1.00	50.19	A
ATOM	3978	CD	GLN	A	533	12.387	11.963	26.783	1.00	50.19	A
ATOM	3979	OE1	GLN	A	533	12.761	11.356	27.798	1.00	50.19	A
ATOM	3980	NE2	GLN	A	533	11.417	11.516	25.997	1.00	50.19	A
ATOM	3981	C	GLN	A	533	16.665	14.473	26.405	1.00	36.89	A
ATOM	3982	O	GLN	A	533	17.049	15.093	27.388	1.00	36.89	A
ATOM	3983	N	VAL	A	534	17.471	13.732	25.651	1.00	41.68	A
ATOM	3984	CA	VAL	A	534	18.895	13.601	25.961	1.00	41.68	A
ATOM	3985	CB	VAL	A	534	19.610	12.666	24.950	1.00	53.57	A
ATOM	3986	CG1	VAL	A	534	21.090	12.544	25.308	1.00	53.57	A
ATOM	3987	CG2	VAL	A	534	18.954	11.292	24.953	1.00	53.57	A
ATOM	3988	C	VAL	A	534	19.560	14.972	25.919	1.00	41.68	A
ATOM	3989	O	VAL	A	534	20.243	15.367	26.854	1.00	41.68	A
ATOM	3990	N	LEU	A	535	19.337	15.694	24.825	1.00	37.41	A
ATOM	3991	CA	LEU	A	535	19.908	17.023	24.639	1.00	37.41	A
ATOM	3992	CB	LEU	A	535	19.413	17.611	23.305	1.00	47.41	A
ATOM	3993	CG	LEU	A	535	20.364	17.677	22.098	1.00	47.41	A
ATOM	3994	CD1	LEU	A	535	21.395	16.577	22.139	1.00	47.41	A
ATOM	3995	CD2	LEU	A	535	19.546	17.624	20.808	1.00	47.41	A
ATOM	3996	C	LEU	A	535	19.575	17.964	25.802	1.00	37.41	A
ATOM	3997	O	LEU	A	535	20.424	18.726	26.256	1.00	37.41	A
ATOM	3998	N	SER	A	536	18.344	17.904	26.297	1.00	36.01	A
ATOM	3999	CA	SER	A	536	17.962	18.779	27.402	1.00	36.01	A
ATOM	4000	CB	SER	A	536	16.444	18.768	27.609	1.00	47.05	A
ATOM	4001	OG	SER	A	536	16.018	17.553	28.181	1.00	47.05	A
ATOM	4002	C	SER	A	536	18.658	18.378	28.699	1.00	36.01	A
ATOM	4003	O	SER	A	536	18.914	19.229	29.559	1.00	36.01	A
ATOM	4004	N	LYS	A	537	18.961	17.088	28.839	1.00	40.88	A
ATOM	4005	CA	LYS	A	537	19.649	16.603	30.030	1.00	40.88	A
ATOM	4006	CB	LYS	A	537	19.630	15.070	30.070	1.00	40.82	A
ATOM	4007	CG	LYS	A	537	18.268	14.540	30.488	1.00	40.82	A
ATOM	4008	CD	LYS	A	537	18.142	13.038	30.420	1.00	40.82	A
ATOM	4009	CE	LYS	A	537	16.717	12.630	30.808	1.00	40.82	A
ATOM	4010	NZ	LYS	A	537	16.435	11.186	30.576	1.00	40.82	A
ATOM	4011	C	LYS	A	537	21.086	17.133	30.051	1.00	40.88	A
ATOM	4012	O	LYS	A	537	21.703	17.227	31.108	1.00	40.88	A
ATOM	4013	N	LEU	A	538	21.591	17.514	28.881	1.00	43.77	A
ATOM	4014	CA	LEU	A	538	22.946	18.036	28.752	1.00	43.77	A
ATOM	4015	CB	LEU	A	538	23.636	17.379	27.553	1.00	42.60	A
ATOM	4016	CG	LEU	A	538	23.637	15.845	27.593	1.00	42.60	A
ATOM	4017	CD1	LEU	A	538	24.172	15.273	26.283	1.00	42.60	A
ATOM	4018	CD2	LEU	A	538	24.464	15.375	28.776	1.00	42.60	A
ATOM	4019	C	LEU	A	538	22.958	19.560	28.585	1.00	43.77	A
ATOM	4020	O	LEU	A	538	23.963	20.136	28.161	1.00	43.77	A
ATOM	4021	N	GLY	A	539	21.837	20.200	28.920	1.00	36.99	A
ATOM	4022	CA	GLY	A	539	21.729	21.649	28.814	1.00	36.99	A
ATOM	4023	C	GLY	A	539	21.835	22.237	27.408	1.00	36.99	A

FIGURE 25 CON'T

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ATOM   4024  O   GLY A 539      22.090  23.431  27.260  1.00 36.99      A
ATOM   4025  N   VAL A 540      21.634  21.429  26.375  1.00 46.64      A
ATOM   4026  CA  VAL A 540      21.734  21.925  25.004  1.00 46.64      A
ATOM   4027  CB  VAL A 540      21.999  20.759  24.022  1.00 44.91      A
ATOM   4028  CG1 VAL A 540      22.014  21.267  22.583  1.00 44.91      A
ATOM   4029  CG2 VAL A 540      23.326  20.097  24.353  1.00 44.91      A
ATOM   4030  C   VAL A 540      20.490  22.695  24.537  1.00 46.64      A
ATOM   4031  O   VAL A 540      19.358  22.224  24.697  1.00 46.64      A
ATOM   4032  N   LYS A 541      20.705  23.891  23.990  1.00 45.20      A
ATOM   4033  CA  LYS A 541      19.612  24.719  23.463  1.00 45.20      A
ATOM   4034  CB  LYS A 541      19.990  26.202  23.512  1.00 50.66      A
ATOM   4035  CG  LYS A 541      19.743  26.869  24.857  1.00 50.66      A
ATOM   4036  CD  LYS A 541      20.490  26.179  25.992  1.00 50.66      A
ATOM   4037  CE  LYS A 541      20.064  26.729  27.344  1.00 50.66      A
ATOM   4038  NZ  LYS A 541      20.719  25.993  28.463  1.00 50.66      A
ATOM   4039  C   LYS A 541      19.407  24.281  22.014  1.00 45.20      A
ATOM   4040  O   LYS A 541      19.873  24.926  21.081  1.00 45.20      A
ATOM   4041  N   TYR A 542      18.694  23.176  21.846  1.00 46.76      A
ATOM   4042  CA  TYR A 542      18.451  22.576  20.546  1.00 46.76      A
ATOM   4043  CB  TYR A 542      18.260  21.078  20.758  1.00 41.50      A
ATOM   4044  CG  TYR A 542      17.064  20.777  21.627  1.00 41.50      A
ATOM   4045  CD1 TYR A 542      15.802  20.558  21.059  1.00 41.50      A
ATOM   4046  CE1 TYR A 542      14.680  20.330  21.857  1.00 41.50      A
ATOM   4047  CD2 TYR A 542      17.176  20.760  23.023  1.00 41.50      A
ATOM   4048  CE2 TYR A 542      16.058  20.534  23.837  1.00 41.50      A
ATOM   4049  CZ  TYR A 542      14.816  20.318  23.246  1.00 41.50      A
ATOM   4050  OH  TYR A 542      13.709  20.078  24.029  1.00 41.50      A
ATOM   4051  C   TYR A 542      17.261  23.148  19.771  1.00 46.76      A
ATOM   4052  O   TYR A 542      16.955  22.697  18.666  1.00 46.76      A
ATOM   4053  N   TYR A 543      16.606  24.147  20.343  1.00 41.18      A
ATOM   4054  CA  TYR A 543      15.436  24.749  19.728  1.00 41.18      A
ATOM   4055  CB  TYR A 543      14.166  24.235  20.429  1.00 43.99      A
ATOM   4056  CG  TYR A 543      14.054  24.688  21.878  1.00 43.99      A
ATOM   4057  CD1 TYR A 543      13.424  25.889  22.211  1.00 43.99      A
ATOM   4058  CE1 TYR A 543      13.402  26.358  23.538  1.00 43.99      A
ATOM   4059  CD2 TYR A 543      14.655  23.951  22.909  1.00 43.99      A
ATOM   4060  CE2 TYR A 543      14.639  24.408  24.233  1.00 43.99      A
ATOM   4061  CZ  TYR A 543      14.018  25.612  24.541  1.00 43.99      A
ATOM   4062  OH  TYR A 543      14.064  26.094  25.841  1.00 43.99      A
ATOM   4063  C   TYR A 543      15.489  26.263  19.864  1.00 41.18      A
ATOM   4064  O   TYR A 543      16.318  26.806  20.601  1.00 41.18      A
ATOM   4065  N   VAL A 544      14.595  26.939  19.147  1.00 45.44      A
ATOM   4066  CA  VAL A 544      14.493  28.388  19.217  1.00 45.44      A
ATOM   4067  CB  VAL A 544      15.125  29.076  17.981  1.00 53.29      A
ATOM   4068  CG1 VAL A 544      14.355  28.716  16.714  1.00 53.29      A
ATOM   4069  CG2 VAL A 544      15.152  30.582  18.191  1.00 53.29      A
ATOM   4070  C   VAL A 544      13.011  28.750  19.327  1.00 45.44      A
ATOM   4071  O   VAL A 544      12.152  28.162  18.664  1.00 45.44      A
ATOM   4072  N   LEU A 545      12.725  29.706  20.197  1.00 52.59      A
ATOM   4073  CA  LEU A 545      11.373  30.162  20.441  1.00 52.59      A
ATOM   4074  CB  LEU A 545      11.173  30.317  21.950  1.00 45.83      A
ATOM   4075  CG  LEU A 545       9.881  30.950  22.447  1.00 45.83      A
ATOM   4076  CD1 LEU A 545       8.682  30.142  21.962  1.00 45.83      A
ATOM   4077  CD2 LEU A 545       9.921  31.021  23.965  1.00 45.83      A
ATOM   4078  C   LEU A 545      11.104  31.488  19.726  1.00 52.59      A
ATOM   4079  O   LEU A 545      11.763  32.495  19.996  1.00 52.59      A
ATOM   4080  N   ASP A 546      10.141  31.475  18.805  1.00 58.10      A
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FIGURE 25 CON'T

ATOM	4081	CA	ASP	A	546	9.771	32.671	18.049	1.00	58.10	A
ATOM	4082	CB	ASP	A	546	9.050	32.281	16.751	1.00	102.17	A
ATOM	4083	CG	ASP	A	546	8.575	33.489	15.952	1.00	102.17	A
ATOM	4084	OD1	ASP	A	546	9.405	34.369	15.642	1.00	102.17	A
ATOM	4085	OD2	ASP	A	546	7.370	33.554	15.627	1.00	102.17	A
ATOM	4086	C	ASP	A	546	8.849	33.480	18.941	1.00	58.10	A
ATOM	4087	O	ASP	A	546	7.680	33.690	18.628	1.00	58.10	A
ATOM	4088	N	TYR	A	547	9.395	33.941	20.058	1.00	54.64	A
ATOM	4089	CA	TYR	A	547	8.615	34.687	21.028	1.00	54.64	A
ATOM	4090	CB	TYR	A	547	7.643	33.722	21.702	1.00	57.57	A
ATOM	4091	CG	TYR	A	547	6.670	34.341	22.672	1.00	57.57	A
ATOM	4092	CD1	TYR	A	547	5.573	35.073	22.219	1.00	57.57	A
ATOM	4093	CE1	TYR	A	547	4.635	35.591	23.112	1.00	57.57	A
ATOM	4094	CD2	TYR	A	547	6.813	34.149	24.041	1.00	57.57	A
ATOM	4095	CE2	TYR	A	547	5.886	34.661	24.941	1.00	57.57	A
ATOM	4096	CZ	TYR	A	547	4.796	35.378	24.472	1.00	57.57	A
ATOM	4097	OH	TYR	A	547	3.855	35.852	25.362	1.00	57.57	A
ATOM	4098	C	TYR	A	547	9.561	35.279	22.063	1.00	54.64	A
ATOM	4099	O	TYR	A	547	10.635	34.735	22.318	1.00	54.64	A
ATOM	4100	N	ARG	A	548	9.179	36.405	22.646	1.00	53.73	A
ATOM	4101	CA	ARG	A	548	9.997	37.023	23.675	1.00	53.73	A
ATOM	4102	CB	ARG	A	548	10.686	38.288	23.162	1.00	110.76	A
ATOM	4103	CG	ARG	A	548	12.106	38.065	22.681	1.00	110.76	A
ATOM	4104	CD	ARG	A	548	12.849	39.386	22.556	1.00	110.76	A
ATOM	4105	NE	ARG	A	548	14.244	39.203	22.164	1.00	110.76	A
ATOM	4106	CZ	ARG	A	548	15.132	38.494	22.855	1.00	110.76	A
ATOM	4107	NH1	ARG	A	548	14.776	37.892	23.983	1.00	110.76	A
ATOM	4108	NH2	ARG	A	548	16.381	38.390	22.421	1.00	110.76	A
ATOM	4109	C	ARG	A	548	9.104	37.372	24.844	1.00	53.73	A
ATOM	4110	O	ARG	A	548	8.063	38.004	24.660	1.00	53.73	A
ATOM	4111	N	PHE	A	549	9.496	36.934	26.039	1.00	47.22	A
ATOM	4112	CA	PHE	A	549	8.731	37.220	27.255	1.00	47.22	A
ATOM	4113	CB	PHE	A	549	9.114	36.247	28.379	1.00	45.14	A
ATOM	4114	CG	PHE	A	549	8.630	34.845	28.154	1.00	45.14	A
ATOM	4115	CD1	PHE	A	549	7.358	34.462	28.564	1.00	45.14	A
ATOM	4116	CD2	PHE	A	549	9.413	33.931	27.465	1.00	45.14	A
ATOM	4117	CE1	PHE	A	549	6.871	33.183	28.281	1.00	45.14	A
ATOM	4118	CE2	PHE	A	549	8.934	32.651	27.175	1.00	45.14	A
ATOM	4119	CZ	PHE	A	549	7.656	32.281	27.585	1.00	45.14	A
ATOM	4120	C	PHE	A	549	9.087	38.630	27.665	1.00	47.22	A
ATOM	4121	O	PHE	A	549	10.247	39.023	27.570	1.00	47.22	A
ATOM	4122	N	ASN	A	550	8.092	39.391	28.108	1.00	51.51	A
ATOM	4123	CA	ASN	A	550	8.305	40.768	28.540	1.00	51.51	A
ATOM	4124	CB	ASN	A	550	6.988	41.554	28.473	1.00	74.53	A
ATOM	4125	CG	ASN	A	550	7.180	43.050	28.694	1.00	74.53	A
ATOM	4126	OD1	ASN	A	550	8.011	43.684	28.046	1.00	74.53	A
ATOM	4127	ND2	ASN	A	550	6.402	43.619	29.607	1.00	74.53	A
ATOM	4128	C	ASN	A	550	8.849	40.769	29.965	1.00	51.51	A
ATOM	4129	O	ASN	A	550	8.351	41.480	30.838	1.00	51.51	A
ATOM	4130	N	TYR	A	551	9.873	39.953	30.193	1.00	56.02	A
ATOM	4131	CA	TYR	A	551	10.503	39.846	31.509	1.00	56.02	A
ATOM	4132	CB	TYR	A	551	9.937	38.659	32.295	1.00	48.15	A
ATOM	4133	CG	TYR	A	551	8.465	38.743	32.614	1.00	48.15	A
ATOM	4134	CD1	TYR	A	551	8.005	39.517	33.680	1.00	48.15	A
ATOM	4135	CE1	TYR	A	551	6.653	39.598	33.972	1.00	48.15	A
ATOM	4136	CD2	TYR	A	551	7.527	38.052	31.847	1.00	48.15	A

FIGURE 25 CON'T

ATOM	4137	CE2	TYR	A	551	6.171	38.131	32.130	1.00	48.15	A
ATOM	4138	CZ	TYR	A	551	5.740	38.905	33.187	1.00	48.15	A
ATOM	4139	OH	TYR	A	551	4.394	39.020	33.443	1.00	48.15	A
ATOM	4140	C	TYR	A	551	11.987	39.606	31.315	1.00	56.02	A
ATOM	4141	O	TYR	A	551	12.418	39.160	30.251	1.00	56.02	A
ATOM	4142	N	ASP	A	552	12.771	39.900	32.343	1.00	47.98	A
ATOM	4143	CA	ASP	A	552	14.207	39.657	32.266	1.00	47.98	A
ATOM	4144	CB	ASP	A	552	14.940	40.449	33.355	1.00	50.83	A
ATOM	4145	CG	ASP	A	552	14.885	41.944	33.115	1.00	50.83	A
ATOM	4146	OD1	ASP	A	552	15.518	42.405	32.153	1.00	50.83	A
ATOM	4147	OD2	ASP	A	552	14.198	42.654	33.876	1.00	50.83	A
ATOM	4148	C	ASP	A	552	14.409	38.160	32.475	1.00	47.98	A
ATOM	4149	O	ASP	A	552	15.180	37.519	31.765	1.00	47.98	A
ATOM	4150	N	TYR	A	553	13.688	37.608	33.446	1.00	44.86	A
ATOM	4151	CA	TYR	A	553	13.776	36.184	33.756	1.00	44.86	A
ATOM	4152	CB	TYR	A	553	14.819	35.948	34.854	1.00	50.87	A
ATOM	4153	CG	TYR	A	553	16.205	36.400	34.482	1.00	50.87	A
ATOM	4154	CD1	TYR	A	553	16.973	35.668	33.585	1.00	50.87	A
ATOM	4155	CE1	TYR	A	553	18.230	36.111	33.186	1.00	50.87	A
ATOM	4156	CD2	TYR	A	553	16.731	37.597	34.985	1.00	50.87	A
ATOM	4157	CE2	TYR	A	553	17.990	38.053	34.590	1.00	50.87	A
ATOM	4158	CZ	TYR	A	553	18.732	37.308	33.690	1.00	50.87	A
ATOM	4159	OH	TYR	A	553	19.969	37.754	33.269	1.00	50.87	A
ATOM	4160	C	TYR	A	553	12.424	35.668	34.245	1.00	44.86	A
ATOM	4161	O	TYR	A	553	11.642	36.411	34.840	1.00	44.86	A
ATOM	4162	N	ILE	A	554	12.134	34.403	33.964	1.00	41.31	A
ATOM	4163	CA	ILE	A	554	10.898	33.812	34.458	1.00	41.31	A
ATOM	4164	CB	ILE	A	554	10.088	33.092	33.356	1.00	44.64	A
ATOM	4165	CG2	ILE	A	554	8.914	32.333	33.993	1.00	44.64	A
ATOM	4166	CG1	ILE	A	554	9.547	34.111	32.343	1.00	44.64	A
ATOM	4167	CD1	ILE	A	554	10.576	34.628	31.369	1.00	44.64	A
ATOM	4168	C	ILE	A	554	11.421	32.801	35.463	1.00	41.31	A
ATOM	4169	O	ILE	A	554	12.253	31.963	35.125	1.00	41.31	A
ATOM	4170	N	ILE	A	555	10.962	32.883	36.703	1.00	39.73	A
ATOM	4171	CA	ILE	A	555	11.471	31.959	37.706	1.00	39.73	A
ATOM	4172	CB	ILE	A	555	12.273	32.730	38.786	1.00	41.36	A
ATOM	4173	CG2	ILE	A	555	12.782	31.776	39.854	1.00	41.36	A
ATOM	4174	CG1	ILE	A	555	13.449	33.467	38.121	1.00	41.36	A
ATOM	4175	CD1	ILE	A	555	14.381	34.168	39.098	1.00	41.36	A
ATOM	4176	C	ILE	A	555	10.433	31.068	38.395	1.00	39.73	A
ATOM	4177	O	ILE	A	555	9.391	31.541	38.834	1.00	39.73	A
ATOM	4178	N	GLY	A	556	10.734	29.768	38.456	1.00	38.06	A
ATOM	4179	CA	GLY	A	556	9.861	28.830	39.132	1.00	38.06	A
ATOM	4180	C	GLY	A	556	10.552	28.428	40.430	1.00	38.06	A
ATOM	4181	O	GLY	A	556	11.771	28.169	40.449	1.00	38.06	A
ATOM	4182	N	ILE	A	557	9.800	28.390	41.522	1.00	45.42	A
ATOM	4183	CA	ILE	A	557	10.366	27.989	42.805	1.00	45.42	A
ATOM	4184	CB	ILE	A	557	10.328	29.128	43.857	1.00	46.97	A
ATOM	4185	CG2	ILE	A	557	11.055	30.371	43.340	1.00	46.97	A
ATOM	4186	CG1	ILE	A	557	8.871	29.445	44.203	1.00	46.97	A
ATOM	4187	CD1	ILE	A	557	8.670	29.999	45.604	1.00	46.97	A
ATOM	4188	C	ILE	A	557	9.541	26.845	43.387	1.00	45.42	A
ATOM	4189	O	ILE	A	557	8.384	26.643	43.009	1.00	45.42	A
ATOM	4190	N	ASP	A	558	10.144	26.105	44.311	1.00	46.09	A
ATOM	4191	CA	ASP	A	558	9.454	25.025	44.989	1.00	46.09	A
ATOM	4192	CB	ASP	A	558	9.761	23.673	44.346	1.00	55.82	A
ATOM	4193	CG	ASP	A	558	8.826	22.585	44.831	1.00	55.82	A

FIGURE 25 CON'T

ATOM	4194	OD1	ASP	A	558	7.601	22.817	44.821	1.00	55.82	A
ATOM	4195	OD2	ASP	A	558	9.298	21.503	45.218	1.00	55.82	A
ATOM	4196	C	ASP	A	558	9.927	25.038	46.432	1.00	46.09	A
ATOM	4197	O	ASP	A	558	11.130	25.077	46.705	1.00	46.09	A
ATOM	4198	N	VAL	A	559	8.979	25.029	47.359	1.00	47.12	A
ATOM	4199	CA	VAL	A	559	9.317	25.051	48.773	1.00	47.12	A
ATOM	4200	CB	VAL	A	559	8.472	26.103	49.531	1.00	49.73	A
ATOM	4201	CG1	VAL	A	559	8.932	26.197	50.984	1.00	49.73	A
ATOM	4202	CG2	VAL	A	559	8.597	27.453	48.847	1.00	49.73	A
ATOM	4203	C	VAL	A	559	9.086	23.682	49.394	1.00	47.12	A
ATOM	4204	O	VAL	A	559	7.951	23.237	49.514	1.00	47.12	A
ATOM	4205	N	ALA	A	560	10.172	23.019	49.785	1.00	57.97	A
ATOM	4206	CA	ALA	A	560	10.089	21.692	50.390	1.00	57.97	A
ATOM	4207	CB	ALA	A	560	9.980	20.627	49.302	1.00	68.19	A
ATOM	4208	C	ALA	A	560	11.325	21.439	51.242	1.00	57.97	A
ATOM	4209	O	ALA	A	560	12.361	21.016	50.733	1.00	57.97	A
ATOM	4210	N	PRO	A	561	11.228	21.686	52.553	1.00	70.30	A
ATOM	4211	CD	PRO	A	561	10.071	22.267	53.252	1.00	81.67	A
ATOM	4212	CA	PRO	A	561	12.347	21.489	53.480	1.00	70.30	A
ATOM	4213	CB	PRO	A	561	11.748	21.883	54.827	1.00	81.67	A
ATOM	4214	CG	PRO	A	561	10.727	22.909	54.445	1.00	81.67	A
ATOM	4215	C	PRO	A	561	12.937	20.078	53.508	1.00	70.30	A
ATOM	4216	O	PRO	A	561	12.214	19.086	53.589	1.00	70.30	A
ATOM	4217	N	MSE	A	562	14.262	20.011	53.450	1.00	71.51	A
ATOM	4218	CA	MSE	A	562	14.990	18.749	53.486	1.00	71.51	A
ATOM	4219	CB	MSE	A	562	15.122	18.184	52.078	1.00	192.18	A
ATOM	4220	CG	MSE	A	562	15.864	19.102	51.136	1.00	192.18	A
ATOM	4221	SE	MSE	A	562	15.628	18.577	49.315	1.00	192.18	A
ATOM	4222	CE	MSE	A	562	14.311	19.882	48.783	1.00	192.18	A
ATOM	4223	C	MSE	A	562	16.377	19.021	54.077	1.00	71.51	A
ATOM	4224	O	MSE	A	562	16.821	20.171	54.130	1.00	71.51	A
ATOM	4225	N	LYS	A	563	17.060	17.973	54.523	1.00	84.31	A
ATOM	4226	CA	LYS	A	563	18.383	18.148	55.106	1.00	84.31	A
ATOM	4227	CB	LYS	A	563	18.360	17.782	56.592	1.00	92.57	A
ATOM	4228	CG	LYS	A	563	19.658	18.069	57.321	1.00	92.57	A
ATOM	4229	CD	LYS	A	563	19.527	17.781	58.806	1.00	92.57	A
ATOM	4230	CE	LYS	A	563	20.819	18.096	59.543	1.00	92.57	A
ATOM	4231	NZ	LYS	A	563	20.672	17.920	61.015	1.00	92.57	A
ATOM	4232	C	LYS	A	563	19.420	17.308	54.382	1.00	84.31	A
ATOM	4233	O	LYS	A	563	19.221	16.115	54.158	1.00	84.31	A
ATOM	4234	N	ARG	A	564	20.530	17.940	54.015	1.00	79.02	A
ATOM	4235	CA	ARG	A	564	21.593	17.246	53.312	1.00	79.02	A
ATOM	4236	CB	ARG	A	564	21.527	17.571	51.821	1.00	67.59	A
ATOM	4237	CG	ARG	A	564	20.213	17.153	51.189	1.00	67.59	A
ATOM	4238	CD	ARG	A	564	20.351	17.014	49.705	1.00	67.59	A
ATOM	4239	NE	ARG	A	564	21.530	16.235	49.353	1.00	67.59	A
ATOM	4240	CZ	ARG	A	564	21.728	15.677	48.164	1.00	67.59	A
ATOM	4241	NH1	ARG	A	564	20.816	15.807	47.207	1.00	67.59	A
ATOM	4242	NH2	ARG	A	564	22.839	14.996	47.929	1.00	67.59	A
ATOM	4243	C	ARG	A	564	22.969	17.590	53.862	1.00	79.02	A
ATOM	4244	O	ARG	A	564	23.174	18.672	54.419	1.00	79.02	A
ATOM	4245	N	SER	A	565	23.899	16.652	53.706	1.00	109.76	A
ATOM	4246	CA	SER	A	565	25.269	16.815	54.177	1.00	109.76	A
ATOM	4247	CB	SER	A	565	26.199	15.892	53.386	1.00	81.52	A
ATOM	4248	OG	SER	A	565	25.831	14.533	53.560	1.00	81.52	A
ATOM	4249	C	SER	A	565	25.732	18.261	54.046	1.00	109.76	A
ATOM	4250	O	SER	A	565	26.018	18.733	52.945	1.00	109.76	A

FIGURE 25 CON'T

ATOM	4251	N	GLU	A	566	25.803	18.958	55.179	1.00168.06	A
ATOM	4252	CA	GLU	A	566	26.215	20.357	55.199	1.00168.06	A
ATOM	4253	CB	GLU	A	566	27.688	20.486	54.794	1.00142.20	A
ATOM	4254	CG	GLU	A	566	28.361	21.807	55.179	1.00142.20	A
ATOM	4255	CD	GLU	A	566	27.672	23.035	54.602	1.00142.20	A
ATOM	4256	OE1	GLU	A	566	26.566	23.381	55.069	1.00142.20	A
ATOM	4257	OE2	GLU	A	566	28.238	23.656	53.677	1.00142.20	A
ATOM	4258	C	GLU	A	566	25.331	21.102	54.203	1.00168.06	A
ATOM	4259	O	GLU	A	566	25.805	21.577	53.170	1.00168.06	A
ATOM	4260	N	GLY	A	567	24.042	21.194	54.513	1.00123.79	A
ATOM	4261	CA	GLY	A	567	23.136	21.873	53.611	1.00123.79	A
ATOM	4262	C	GLY	A	567	21.833	22.364	54.206	1.00123.79	A
ATOM	4263	O	GLY	A	567	21.628	23.572	54.317	1.00123.79	A
ATOM	4264	N	TYR	A	568	20.952	21.442	54.593	1.00 77.07	A
ATOM	4265	CA	TYR	A	568	19.649	21.820	55.143	1.00 77.07	A
ATOM	4266	CB	TYR	A	568	19.824	22.493	56.508	1.00128.97	A
ATOM	4267	CG	TYR	A	568	18.536	22.699	57.276	1.00128.97	A
ATOM	4268	CD1	TYR	A	568	18.557	22.938	58.650	1.00128.97	A
ATOM	4269	CE1	TYR	A	568	17.379	23.148	59.362	1.00128.97	A
ATOM	4270	CD2	TYR	A	568	17.299	22.675	56.631	1.00128.97	A
ATOM	4271	CE2	TYR	A	568	16.115	22.885	57.332	1.00128.97	A
ATOM	4272	CZ	TYR	A	568	16.162	23.121	58.697	1.00128.97	A
ATOM	4273	OH	TYR	A	568	14.993	23.337	59.392	1.00128.97	A
ATOM	4274	C	TYR	A	568	19.027	22.783	54.123	1.00 77.07	A
ATOM	4275	O	TYR	A	568	19.068	24.002	54.283	1.00 77.07	A
ATOM	4276	N	ILE	A	569	18.454	22.210	53.070	1.00 62.58	A
ATOM	4277	CA	ILE	A	569	17.874	22.986	51.984	1.00 62.58	A
ATOM	4278	CB	ILE	A	569	18.214	22.331	50.642	1.00 78.12	A
ATOM	4279	CG2	ILE	A	569	17.748	23.211	49.491	1.00 78.12	A
ATOM	4280	CG1	ILE	A	569	19.727	22.110	50.571	1.00 78.12	A
ATOM	4281	CD1	ILE	A	569	20.195	21.387	49.332	1.00 78.12	A
ATOM	4282	C	ILE	A	569	16.375	23.197	52.086	1.00 62.58	A
ATOM	4283	O	ILE	A	569	15.614	22.269	52.353	1.00 62.58	A
ATOM	4284	N	GLY	A	570	15.958	24.436	51.852	1.00 48.55	A
ATOM	4285	CA	GLY	A	570	14.549	24.769	51.941	1.00 48.55	A
ATOM	4286	C	GLY	A	570	13.752	24.635	50.656	1.00 48.55	A
ATOM	4287	O	GLY	A	570	12.531	24.732	50.684	1.00 48.55	A
ATOM	4288	N	GLY	A	571	14.427	24.419	49.532	1.00 44.27	A
ATOM	4289	CA	GLY	A	571	13.704	24.286	48.280	1.00 44.27	A
ATOM	4290	C	GLY	A	571	14.565	24.498	47.062	1.00 44.27	A
ATOM	4291	O	GLY	A	571	15.780	24.288	47.094	1.00 44.27	A
ATOM	4292	N	SER	A	572	13.951	24.952	45.980	1.00 40.81	A
ATOM	4293	CA	SER	A	572	14.703	25.145	44.758	1.00 40.81	A
ATOM	4294	CB	SER	A	572	14.616	23.878	43.920	1.00 44.63	A
ATOM	4295	OG	SER	A	572	13.279	23.716	43.480	1.00 44.63	A
ATOM	4296	C	SER	A	572	14.169	26.302	43.935	1.00 40.81	A
ATOM	4297	O	SER	A	572	13.168	26.917	44.289	1.00 40.81	A
ATOM	4298	N	ALA	A	573	14.848	26.577	42.823	1.00 45.14	A
ATOM	4299	CA	ALA	A	573	14.443	27.638	41.908	1.00 45.14	A
ATOM	4300	CB	ALA	A	573	14.930	29.008	42.407	1.00 42.74	A
ATOM	4301	C	ALA	A	573	15.027	27.349	40.537	1.00 45.14	A
ATOM	4302	O	ALA	A	573	16.190	26.943	40.413	1.00 45.14	A
ATOM	4303	N	VAL	A	574	14.211	27.541	39.510	1.00 43.22	A
ATOM	4304	CA	VAL	A	574	14.645	27.319	38.144	1.00 43.22	A
ATOM	4305	CB	VAL	A	574	13.914	26.131	37.501	1.00 36.40	A
ATOM	4306	CG1	VAL	A	574	14.371	25.970	36.053	1.00 36.40	A

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ATOM	4307	CG2	VAL	A	574	14.198	24.859	38.295	1.00	36.40	A
ATOM	4308	C	VAL	A	574	14.385	28.586	37.336	1.00	43.22	A
ATOM	4309	O	VAL	A	574	13.285	29.139	37.336	1.00	43.22	A
ATOM	4310	N	MSE	A	575	15.413	29.022	36.628	1.00	37.32	A
ATOM	4311	CA	MSE	A	575	15.354	30.247	35.860	1.00	37.32	A
ATOM	4312	CB	MSE	A	575	16.475	31.169	36.363	1.00	58.88	A
ATOM	4313	CG	MSE	A	575	16.679	32.475	35.609	1.00	58.88	A
ATOM	4314	SE	MSE	A	575	18.345	33.372	36.183	1.00	58.88	A
ATOM	4315	CE	MSE	A	575	19.467	32.802	34.741	1.00	58.88	A
ATOM	4316	C	MSE	A	575	15.461	30.070	34.355	1.00	37.32	A
ATOM	4317	O	MSE	A	575	16.314	29.335	33.862	1.00	37.32	A
ATOM	4318	N	PHE	A	576	14.581	30.768	33.640	1.00	37.08	A
ATOM	4319	CA	PHE	A	576	14.567	30.785	32.179	1.00	37.08	A
ATOM	4320	CB	PHE	A	576	13.195	30.352	31.631	1.00	38.91	A
ATOM	4321	CG	PHE	A	576	12.965	28.870	31.651	1.00	38.91	A
ATOM	4322	CD1	PHE	A	576	12.744	28.179	30.466	1.00	38.91	A
ATOM	4323	CD2	PHE	A	576	12.926	28.173	32.854	1.00	38.91	A
ATOM	4324	CE1	PHE	A	576	12.482	26.818	30.472	1.00	38.91	A
ATOM	4325	CE2	PHE	A	576	12.662	26.799	32.872	1.00	38.91	A
ATOM	4326	CZ	PHE	A	576	12.438	26.124	31.685	1.00	38.91	A
ATOM	4327	C	PHE	A	576	14.791	32.243	31.785	1.00	37.08	A
ATOM	4328	O	PHE	A	576	14.442	33.139	32.548	1.00	37.08	A
ATOM	4329	N	ASP	A	577	15.357	32.489	30.607	1.00	47.44	A
ATOM	4330	CA	ASP	A	577	15.559	33.866	30.170	1.00	47.44	A
ATOM	4331	CB	ASP	A	577	16.885	34.011	29.397	1.00	45.16	A
ATOM	4332	CG	ASP	A	577	16.962	33.106	28.192	1.00	45.16	A
ATOM	4333	OD1	ASP	A	577	15.896	32.724	27.661	1.00	45.16	A
ATOM	4334	OD2	ASP	A	577	18.087	32.780	27.756	1.00	45.16	A
ATOM	4335	C	ASP	A	577	14.357	34.264	29.296	1.00	47.44	A
ATOM	4336	O	ASP	A	577	13.490	33.431	29.004	1.00	47.44	A
ATOM	4337	N	SER	A	578	14.293	35.523	28.878	1.00	48.69	A
ATOM	4338	CA	SER	A	578	13.160	35.992	28.071	1.00	48.69	A
ATOM	4339	CB	SER	A	578	13.271	37.500	27.826	1.00	56.23	A
ATOM	4340	OG	SER	A	578	14.368	37.803	26.983	1.00	56.23	A
ATOM	4341	C	SER	A	578	13.046	35.270	26.735	1.00	48.69	A
ATOM	4342	O	SER	A	578	12.042	35.392	26.029	1.00	48.69	A
ATOM	4343	N	GLN	A	579	14.076	34.505	26.399	1.00	44.48	A
ATOM	4344	CA	GLN	A	579	14.106	33.776	25.140	1.00	44.48	A
ATOM	4345	CB	GLN	A	579	15.543	33.730	24.627	1.00	84.17	A
ATOM	4346	CG	GLN	A	579	15.676	33.788	23.126	1.00	84.17	A
ATOM	4347	CD	GLN	A	579	17.112	33.619	22.676	1.00	84.17	A
ATOM	4348	OE1	GLN	A	579	18.022	34.253	23.215	1.00	84.17	A
ATOM	4349	NE2	GLN	A	579	17.323	32.767	21.679	1.00	84.17	A
ATOM	4350	C	GLN	A	579	13.557	32.345	25.275	1.00	44.48	A
ATOM	4351	O	GLN	A	579	13.575	31.576	24.315	1.00	44.48	A
ATOM	4352	N	GLY	A	580	13.078	31.983	26.460	1.00	38.30	A
ATOM	4353	CA	GLY	A	580	12.540	30.645	26.632	1.00	38.30	A
ATOM	4354	C	GLY	A	580	13.553	29.530	26.859	1.00	38.30	A
ATOM	4355	O	GLY	A	580	13.243	28.347	26.639	1.00	38.30	A
ATOM	4356	N	TYR	A	581	14.766	29.895	27.275	1.00	45.22	A
ATOM	4357	CA	TYR	A	581	15.797	28.898	27.557	1.00	45.22	A
ATOM	4358	CB	TYR	A	581	17.122	29.245	26.883	1.00	50.66	A
ATOM	4359	CG	TYR	A	581	17.105	29.220	25.377	1.00	50.66	A
ATOM	4360	CD1	TYR	A	581	16.611	28.118	24.682	1.00	50.66	A
ATOM	4361	CE1	TYR	A	581	16.641	28.073	23.289	1.00	50.66	A
ATOM	4362	CD2	TYR	A	581	17.626	30.288	24.642	1.00	50.66	A
ATOM	4363	CE2	TYR	A	581	17.662	30.256	23.253	1.00	50.66	A

ATOM	4364	CZ	TYR	A	581	17.171	29.144	22.583	1.00	50.66	A
ATOM	4365	OH	TYR	A	581	17.239	29.092	21.210	1.00	50.66	A
ATOM	4366	C	TYR	A	581	16.049	28.811	29.050	1.00	45.22	A
ATOM	4367	O	TYR	A	581	16.106	29.829	29.749	1.00	45.22	A
ATOM	4368	N	ILE	A	582	16.195	27.592	29.545	1.00	39.10	A
ATOM	4369	CA	ILE	A	582	16.486	27.397	30.960	1.00	39.10	A
ATOM	4370	CB	ILE	A	582	16.203	25.924	31.370	1.00	41.87	A
ATOM	4371	CG2	ILE	A	582	16.939	24.967	30.446	1.00	41.87	A
ATOM	4372	CG1	ILE	A	582	16.608	25.678	32.821	1.00	41.87	A
ATOM	4373	CD1	ILE	A	582	16.159	24.302	33.326	1.00	41.87	A
ATOM	4374	C	ILE	A	582	17.976	27.751	31.112	1.00	39.10	A
ATOM	4375	O	ILE	A	582	18.798	27.333	30.308	1.00	39.10	A
ATOM	4376	N	ARG	A	583	18.328	28.528	32.124	1.00	43.00	A
ATOM	4377	CA	ARG	A	583	19.731	28.909	32.279	1.00	43.00	A
ATOM	4378	CB	ARG	A	583	19.878	30.428	32.140	1.00	57.85	A
ATOM	4379	CG	ARG	A	583	18.911	31.025	31.134	1.00	57.85	A
ATOM	4380	CD	ARG	A	583	19.573	31.571	29.879	1.00	57.85	A
ATOM	4381	NE	ARG	A	583	20.420	30.619	29.168	1.00	57.85	A
ATOM	4382	CZ	ARG	A	583	20.704	30.709	27.866	1.00	57.85	A
ATOM	4383	NH1	ARG	A	583	20.195	31.696	27.143	1.00	57.85	A
ATOM	4384	NH2	ARG	A	583	21.528	29.838	27.293	1.00	57.85	A
ATOM	4385	C	ARG	A	583	20.348	28.465	33.595	1.00	43.00	A
ATOM	4386	O	ARG	A	583	21.500	28.036	33.624	1.00	43.00	A
ATOM	4387	N	LYS	A	584	19.579	28.561	34.677	1.00	44.21	A
ATOM	4388	CA	LYS	A	584	20.079	28.188	35.992	1.00	44.21	A
ATOM	4389	CB	LYS	A	584	20.504	29.450	36.749	1.00	51.60	A
ATOM	4390	CG	LYS	A	584	21.413	30.410	35.971	1.00	51.60	A
ATOM	4391	CD	LYS	A	584	22.796	29.849	35.715	1.00	51.60	A
ATOM	4392	CE	LYS	A	584	23.693	30.901	35.057	1.00	51.60	A
ATOM	4393	NZ	LYS	A	584	25.007	30.344	34.614	1.00	51.60	A
ATOM	4394	C	LYS	A	584	19.085	27.399	36.858	1.00	44.21	A
ATOM	4395	O	LYS	A	584	17.878	27.687	36.886	1.00	44.21	A
ATOM	4396	N	ILE	A	585	19.627	26.419	37.582	1.00	42.37	A
ATOM	4397	CA	ILE	A	585	18.870	25.565	38.489	1.00	42.37	A
ATOM	4398	CB	ILE	A	585	18.807	24.124	37.953	1.00	38.40	A
ATOM	4399	CG2	ILE	A	585	18.059	23.225	38.948	1.00	38.40	A
ATOM	4400	CG1	ILE	A	585	18.146	24.132	36.569	1.00	38.40	A
ATOM	4401	CD1	ILE	A	585	18.160	22.800	35.879	1.00	38.40	A
ATOM	4402	C	ILE	A	585	19.606	25.571	39.826	1.00	42.37	A
ATOM	4403	O	ILE	A	585	20.752	25.148	39.901	1.00	42.37	A
ATOM	4404	N	VAL	A	586	18.950	26.015	40.888	1.00	41.24	A
ATOM	4405	CA	VAL	A	586	19.631	26.090	42.175	1.00	41.24	A
ATOM	4406	CB	VAL	A	586	20.043	27.540	42.500	1.00	41.89	A
ATOM	4407	CG1	VAL	A	586	20.986	28.081	41.441	1.00	41.89	A
ATOM	4408	CG2	VAL	A	586	18.798	28.397	42.617	1.00	41.89	A
ATOM	4409	C	VAL	A	586	18.914	25.595	43.419	1.00	41.24	A
ATOM	4410	O	VAL	A	586	17.692	25.641	43.515	1.00	41.24	A
ATOM	4411	N	PRO	A	587	19.691	25.124	44.406	1.00	43.78	A
ATOM	4412	CD	PRO	A	587	21.128	24.818	44.331	1.00	58.45	A
ATOM	4413	CA	PRO	A	587	19.129	24.637	45.665	1.00	43.78	A
ATOM	4414	CB	PRO	A	587	20.219	23.709	46.213	1.00	58.45	A
ATOM	4415	CG	PRO	A	587	21.191	23.522	45.071	1.00	58.45	A
ATOM	4416	C	PRO	A	587	19.019	25.890	46.515	1.00	43.78	A
ATOM	4417	O	PRO	A	587	19.749	26.850	46.284	1.00	43.78	A
ATOM	4418	N	ILE	A	588	18.128	25.905	47.490	1.00	53.06	A
ATOM	4419	CA	ILE	A	588	18.027	27.080	48.328	1.00	53.06	A

ATOM	4420	CB	ILE	A	588	16.652	27.763	48.170	1.00	53.55	A
ATOM	4421	CG2	ILE	A	588	16.546	28.980	49.090	1.00	53.55	A
ATOM	4422	CG1	ILE	A	588	16.492	28.194	46.710	1.00	53.55	A
ATOM	4423	CD1	ILE	A	588	15.412	29.187	46.476	1.00	53.55	A
ATOM	4424	C	ILE	A	588	18.316	26.727	49.778	1.00	53.06	A
ATOM	4425	O	ILE	A	588	17.439	26.299	50.539	1.00	53.06	A
ATOM	4426	N	LYS	A	589	19.581	26.906	50.137	1.00	62.38	A
ATOM	4427	CA	LYS	A	589	20.072	26.620	51.477	1.00	62.38	A
ATOM	4428	CB	LYS	A	589	21.593	26.795	51.491	1.00	98.66	A
ATOM	4429	CG	LYS	A	589	22.333	26.038	52.573	1.00	98.66	A
ATOM	4430	CD	LYS	A	589	23.836	26.163	52.362	1.00	98.66	A
ATOM	4431	CE	LYS	A	589	24.615	25.273	53.314	1.00	98.66	A
ATOM	4432	NZ	LYS	A	589	24.361	25.631	54.734	1.00	98.66	A
ATOM	4433	C	LYS	A	589	19.414	27.593	52.455	1.00	62.38	A
ATOM	4434	O	LYS	A	589	19.259	28.773	52.152	1.00	62.38	A
ATOM	4435	N	ILE	A	590	18.998	27.090	53.612	1.00	72.19	A
ATOM	4436	CA	ILE	A	590	18.379	27.934	54.628	1.00	72.19	A
ATOM	4437	CB	ILE	A	590	16.836	27.921	54.540	1.00	70.84	A
ATOM	4438	CG2	ILE	A	590	16.387	28.396	53.168	1.00	70.84	A
ATOM	4439	CG1	ILE	A	590	16.306	26.514	54.820	1.00	70.84	A
ATOM	4440	CD1	ILE	A	590	14.797	26.441	54.917	1.00	70.84	A
ATOM	4441	C	ILE	A	590	18.787	27.418	56.001	1.00	72.19	A
ATOM	4442	O	ILE	A	590	19.033	26.225	56.171	1.00	72.19	A
ATOM	4443	N	GLY	A	591	18.871	28.318	56.974	1.00	74.83	A
ATOM	4444	CA	GLY	A	591	19.245	27.908	58.315	1.00	74.83	A
ATOM	4445	C	GLY	A	591	18.101	27.164	58.978	1.00	74.83	A
ATOM	4446	O	GLY	A	591	17.047	26.971	58.370	1.00	74.83	A
ATOM	4447	N	GLU	A	592	18.304	26.740	60.222	1.00	110.79	A
ATOM	4448	CA	GLU	A	592	17.268	26.026	60.957	1.00	110.79	A
ATOM	4449	CB	GLU	A	592	17.799	25.558	62.314	1.00	154.33	A
ATOM	4450	CG	GLU	A	592	16.773	24.804	63.144	1.00	154.33	A
ATOM	4451	CD	GLU	A	592	17.318	24.356	64.484	1.00	154.33	A
ATOM	4452	OE1	GLU	A	592	17.770	25.220	65.264	1.00	154.33	A
ATOM	4453	OE2	GLU	A	592	17.291	23.138	64.758	1.00	154.33	A
ATOM	4454	C	GLU	A	592	16.065	26.941	61.160	1.00	110.79	A
ATOM	4455	O	GLU	A	592	16.218	28.121	61.476	1.00	110.79	A
ATOM	4456	N	GLN	A	593	14.870	26.389	60.981	1.00	105.70	A
ATOM	4457	CA	GLN	A	593	13.642	27.158	61.126	1.00	105.70	A
ATOM	4458	CB	GLN	A	593	12.499	26.465	60.388	1.00	172.39	A
ATOM	4459	CG	GLN	A	593	12.853	26.007	58.992	1.00	172.39	A
ATOM	4460	CD	GLN	A	593	11.657	25.464	58.245	1.00	172.39	A
ATOM	4461	OE1	GLN	A	593	10.979	24.546	58.710	1.00	172.39	A
ATOM	4462	NE2	GLN	A	593	11.389	26.030	57.078	1.00	172.39	A
ATOM	4463	C	GLN	A	593	13.243	27.347	62.581	1.00	105.70	A
ATOM	4464	O	GLN	A	593	13.261	26.400	63.366	1.00	105.70	A
ATOM	4465	N	ARG	A	594	12.877	28.577	62.931	1.00	112.07	A
ATOM	4466	CA	ARG	A	594	12.452	28.887	64.289	1.00	112.07	A
ATOM	4467	CB	ARG	A	594	12.507	30.397	64.534	1.00	153.19	A
ATOM	4468	CG	ARG	A	594	13.915	30.955	64.660	1.00	153.19	A
ATOM	4469	CD	ARG	A	594	14.653	30.313	65.827	1.00	153.19	A
ATOM	4470	NE	ARG	A	594	15.966	30.911	66.051	1.00	153.19	A
ATOM	4471	CZ	ARG	A	594	16.160	32.179	66.401	1.00	153.19	A
ATOM	4472	NH1	ARG	A	594	15.123	32.990	66.569	1.00	153.19	A
ATOM	4473	NH2	ARG	A	594	17.391	32.637	66.587	1.00	153.19	A
ATOM	4474	C	ARG	A	594	11.031	28.377	64.496	1.00	112.07	A
ATOM	4475	O	ARG	A	594	10.823	27.325	65.102	1.00	112.07	A
ATOM	4476	N	GLY	A	595	10.056	29.125	63.989	1.00	111.54	A

FIGURE 25 CON'T

ATOM	4477	CA	GLY	A	595	8.670	28.715	64.124	1.00111.54	A
ATOM	4478	C	GLY	A	595	8.327	27.654	63.097	1.00111.54	A
ATOM	4479	O	GLY	A	595	9.098	27.413	62.169	1.00111.54	A
ATOM	4480	N	GLU	A	596	7.177	27.008	63.261	1.00136.15	A
ATOM	4481	CA	GLU	A	596	6.756	25.978	62.320	1.00136.15	A
ATOM	4482	CB	GLU	A	596	5.620	25.139	62.916	1.00144.37	A
ATOM	4483	CG	GLU	A	596	6.072	24.148	63.984	1.00144.37	A
ATOM	4484	CD	GLU	A	596	6.946	23.037	63.422	1.00144.37	A
ATOM	4485	OE1	GLU	A	596	6.460	22.274	62.561	1.00144.37	A
ATOM	4486	OE2	GLU	A	596	8.117	22.925	63.841	1.00144.37	A
ATOM	4487	C	GLU	A	596	6.306	26.621	61.014	1.00136.15	A
ATOM	4488	O	GLU	A	596	5.124	26.602	60.668	1.00136.15	A
ATOM	4489	N	SER	A	597	7.269	27.193	60.297	1.00115.88	A
ATOM	4490	CA	SER	A	597	7.016	27.857	59.024	1.00115.88	A
ATOM	4491	CB	SER	A	597	6.091	29.057	59.227	1.00 95.41	A
ATOM	4492	OG	SER	A	597	5.873	29.737	58.005	1.00 95.41	A
ATOM	4493	C	SER	A	597	8.336	28.324	58.420	1.00115.88	A
ATOM	4494	O	SER	A	597	9.210	28.825	59.129	1.00115.88	A
ATOM	4495	N	VAL	A	598	8.479	28.157	57.109	1.00 68.76	A
ATOM	4496	CA	VAL	A	598	9.701	28.560	56.419	1.00 68.76	A
ATOM	4497	CB	VAL	A	598	9.765	27.967	54.994	1.00 80.99	A
ATOM	4498	CG1	VAL	A	598	11.110	28.287	54.359	1.00 80.99	A
ATOM	4499	CG2	VAL	A	598	9.529	26.467	55.040	1.00 80.99	A
ATOM	4500	C	VAL	A	598	9.786	30.078	56.301	1.00 68.76	A
ATOM	4501	O	VAL	A	598	8.816	30.728	55.912	1.00 68.76	A
ATOM	4502	N	ASP	A	599	10.945	30.640	56.638	1.00 53.04	A
ATOM	4503	CA	ASP	A	599	11.143	32.086	56.545	1.00 53.04	A
ATOM	4504	CB	ASP	A	599	12.340	32.528	57.392	1.00 72.22	A
ATOM	4505	CG	ASP	A	599	12.561	34.032	57.343	1.00 72.22	A
ATOM	4506	OD1	ASP	A	599	12.782	34.574	56.241	1.00 72.22	A
ATOM	4507	OD2	ASP	A	599	12.509	34.678	58.406	1.00 72.22	A
ATOM	4508	C	ASP	A	599	11.386	32.462	55.087	1.00 53.04	A
ATOM	4509	O	ASP	A	599	12.518	32.393	54.589	1.00 53.04	A
ATOM	4510	N	MSE	A	600	10.323	32.878	54.408	1.00 59.23	A
ATOM	4511	CA	MSE	A	600	10.425	33.230	53.003	1.00 59.23	A
ATOM	4512	CB	MSE	A	600	9.028	33.456	52.423	1.00 57.98	A
ATOM	4513	CG	MSE	A	600	8.137	32.205	52.487	1.00 57.98	A
ATOM	4514	SE	MSE	A	600	9.060	30.559	51.959	1.00 57.98	A
ATOM	4515	CE	MSE	A	600	9.289	30.938	50.077	1.00 57.98	A
ATOM	4516	C	MSE	A	600	11.343	34.416	52.722	1.00 59.23	A
ATOM	4517	O	MSE	A	600	11.885	34.536	51.617	1.00 59.23	A
ATOM	4518	N	ASN	A	601	11.538	35.287	53.710	1.00 51.21	A
ATOM	4519	CA	ASN	A	601	12.439	36.419	53.509	1.00 51.21	A
ATOM	4520	CB	ASN	A	601	12.405	37.363	54.714	1.00 78.56	A
ATOM	4521	CG	ASN	A	601	11.075	38.079	54.854	1.00 78.56	A
ATOM	4522	OD1	ASN	A	601	10.591	38.698	53.909	1.00 78.56	A
ATOM	4523	ND2	ASN	A	601	10.478	37.998	56.037	1.00 78.56	A
ATOM	4524	C	ASN	A	601	13.836	35.842	53.319	1.00 51.21	A
ATOM	4525	O	ASN	A	601	14.568	36.230	52.407	1.00 51.21	A
ATOM	4526	N	GLU	A	602	14.190	34.885	54.168	1.00 50.53	A
ATOM	4527	CA	GLU	A	602	15.499	34.238	54.087	1.00 50.53	A
ATOM	4528	CB	GLU	A	602	15.696	33.313	55.291	1.00 60.76	A
ATOM	4529	CG	GLU	A	602	17.076	32.672	55.381	1.00 60.76	A
ATOM	4530	CD	GLU	A	602	17.148	31.600	56.455	1.00 60.76	A
ATOM	4531	OE1	GLU	A	602	16.220	31.533	57.287	1.00 60.76	A
ATOM	4532	OE2	GLU	A	602	18.131	30.831	56.472	1.00 60.76	A

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ATOM   4533  C   GLU A 602      15.579  33.424  52.792  1.00 50.53      A
ATOM   4534  O   GLU A 602      16.592  33.434  52.101  1.00 50.53      A
ATOM   4535  N   PHE A 603      14.490  32.729  52.475  1.00 50.35      A
ATOM   4536  CA  PHE A 603      14.403  31.898  51.277  1.00 50.35      A
ATOM   4537  CB  PHE A 603      12.987  31.302  51.178  1.00 52.94      A
ATOM   4538  CG  PHE A 603      12.818  30.288  50.075  1.00 52.94      A
ATOM   4539  CD1 PHE A 603      12.777  28.925  50.364  1.00 52.94      A
ATOM   4540  CD2 PHE A 603      12.687  30.692  48.750  1.00 52.94      A
ATOM   4541  CE1 PHE A 603      12.606  27.983  49.355  1.00 52.94      A
ATOM   4542  CE2 PHE A 603      12.515  29.749  47.727  1.00 52.94      A
ATOM   4543  CZ  PHE A 603      12.474  28.393  48.033  1.00 52.94      A
ATOM   4544  C   PHE A 603      14.725  32.689  50.003  1.00 50.35      A
ATOM   4545  O   PHE A 603      15.664  32.370  49.276  1.00 50.35      A
ATOM   4546  N   PHE A 604      13.940  33.722  49.729  1.00 46.12      A
ATOM   4547  CA  PHE A 604      14.152  34.524  48.537  1.00 46.12      A
ATOM   4548  CB  PHE A 604      12.981  35.500  48.353  1.00 50.73      A
ATOM   4549  CG  PHE A 604      11.672  34.816  48.010  1.00 50.73      A
ATOM   4550  CD1 PHE A 604      11.547  34.065  46.840  1.00 50.73      A
ATOM   4551  CD2 PHE A 604      10.574  34.910  48.857  1.00 50.73      A
ATOM   4552  CE1 PHE A 604      10.343  33.415  46.515  1.00 50.73      A
ATOM   4553  CE2 PHE A 604       9.368  34.262  48.542  1.00 50.73      A
ATOM   4554  CZ  PHE A 604       9.258  33.512  47.363  1.00 50.73      A
ATOM   4555  C   PHE A 604      15.496  35.256  48.559  1.00 46.12      A
ATOM   4556  O   PHE A 604      16.168  35.378  47.524  1.00 46.12      A
ATOM   4557  N   LYS A 605      15.909  35.728  49.729  1.00 56.20      A
ATOM   4558  CA  LYS A 605      17.194  36.409  49.807  1.00 56.20      A
ATOM   4559  CB  LYS A 605      17.469  36.883  51.240  1.00 83.58      A
ATOM   4560  CG  LYS A 605      18.801  37.594  51.407  1.00 83.58      A
ATOM   4561  CD  LYS A 605      18.921  38.256  52.777  1.00 83.58      A
ATOM   4562  CE  LYS A 605      20.381  38.484  53.161  1.00 83.58      A
ATOM   4563  NZ  LYS A 605      21.157  39.164  52.089  1.00 83.58      A
ATOM   4564  C   LYS A 605      18.263  35.416  49.344  1.00 56.20      A
ATOM   4565  O   LYS A 605      19.134  35.757  48.530  1.00 56.20      A
ATOM   4566  N   GLU A 606      18.189  34.182  49.846  1.00 44.36      A
ATOM   4567  CA  GLU A 606      19.157  33.172  49.427  1.00 44.36      A
ATOM   4568  CB  GLU A 606      18.997  31.885  50.236  1.00 58.25      A
ATOM   4569  CG  GLU A 606      19.884  30.744  49.730  1.00 58.25      A
ATOM   4570  CD  GLU A 606      21.359  31.118  49.680  1.00 58.25      A
ATOM   4571  OE1 GLU A 606      22.149  30.371  49.060  1.00 58.25      A
ATOM   4572  OE2 GLU A 606      21.734  32.159  50.262  1.00 58.25      A
ATOM   4573  C   GLU A 606      19.010  32.860  47.934  1.00 44.36      A
ATOM   4574  O   GLU A 606      19.998  32.566  47.253  1.00 44.36      A
ATOM   4575  N   MSE A 607      17.785  32.931  47.419  1.00 52.22      A
ATOM   4576  CA  MSE A 607      17.565  32.650  45.999  1.00 52.22      A
ATOM   4577  CB  MSE A 607      16.074  32.745  45.648  1.00 47.94      A
ATOM   4578  CG  MSE A 607      15.778  32.490  44.171  1.00 47.94      A
ATOM   4579  SE  MSE A 607      13.931  32.858  43.696  1.00 47.94      A
ATOM   4580  CE  MSE A 607      14.062  34.789  43.491  1.00 47.94      A
ATOM   4581  C   MSE A 607      18.353  33.651  45.159  1.00 52.22      A
ATOM   4582  O   MSE A 607      19.067  33.276  44.221  1.00 52.22      A
ATOM   4583  N   VAL A 608      18.216  34.929  45.507  1.00 49.17      A
ATOM   4584  CA  VAL A 608      18.917  35.996  44.804  1.00 49.17      A
ATOM   4585  CB  VAL A 608      18.492  37.375  45.342  1.00 62.97      A
ATOM   4586  CG1 VAL A 608      19.453  38.456  44.855  1.00 62.97      A
ATOM   4587  CG2 VAL A 608      17.091  37.686  44.867  1.00 62.97      A
ATOM   4588  C   VAL A 608      20.431  35.844  44.933  1.00 49.17      A
ATOM   4589  O   VAL A 608      21.162  35.933  43.945  1.00 49.17      A
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FIGURE 25 CON'T

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ATOM   4590  N   ASP A 609      20.902  35.600  46.148  1.00 54.49      A
ATOM   4591  CA  ASP A 609      22.333  35.433  46.366  1.00 54.49      A
ATOM   4592  CB  ASP A 609      22.641  35.350  47.862  1.00 60.18      A
ATOM   4593  CG  ASP A 609      22.438  36.673  48.573  1.00 60.18      A
ATOM   4594  OD1 ASP A 609      22.339  37.710  47.883  1.00 66.27      A
ATOM   4595  OD2 ASP A 609      22.378  36.675  49.821  1.00 66.27      A
ATOM   4596  C   ASP A 609      22.865  34.203  45.650  1.00 54.49      A
ATOM   4597  O   ASP A 609      23.970  34.228  45.096  1.00 54.49      A
ATOM   4598  N   LYS A 610      22.079  33.126  45.639  1.00 51.28      A
ATOM   4599  CA  LYS A 610      22.524  31.906  44.973  1.00 51.28      A
ATOM   4600  CB  LYS A 610      21.566  30.753  45.263  1.00 62.45      A
ATOM   4601  CG  LYS A 610      22.154  29.394  44.925  1.00 62.45      A
ATOM   4602  CD  LYS A 610      23.396  29.146  45.766  1.00 62.45      A
ATOM   4603  CE  LYS A 610      23.815  27.691  45.761  1.00 62.45      A
ATOM   4604  NZ  LYS A 610      24.296  27.265  44.431  1.00 62.45      A
ATOM   4605  C   LYS A 610      22.652  32.108  43.463  1.00 51.28      A
ATOM   4606  O   LYS A 610      23.611  31.641  42.848  1.00 51.28      A
ATOM   4607  N   PHE A 611      21.687  32.794  42.857  1.00 48.60      A
ATOM   4608  CA  PHE A 611      21.768  33.033  41.417  1.00 48.60      A
ATOM   4609  CB  PHE A 611      20.502  33.728  40.900  1.00 48.45      A
ATOM   4610  CG  PHE A 611      19.338  32.790  40.684  1.00 48.45      A
ATOM   4611  CD1 PHE A 611      19.473  31.669  39.867  1.00 48.45      A
ATOM   4612  CD2 PHE A 611      18.107  33.037  41.283  1.00 48.45      A
ATOM   4613  CE1 PHE A 611      18.392  30.799  39.646  1.00 48.45      A
ATOM   4614  CE2 PHE A 611      17.021  32.181  41.074  1.00 48.45      A
ATOM   4615  CZ  PHE A 611      17.163  31.055  40.251  1.00 48.45      A
ATOM   4616  C   PHE A 611      22.999  33.874  41.107  1.00 48.60      A
ATOM   4617  O   PHE A 611      23.663  33.672  40.085  1.00 48.60      A
ATOM   4618  N   LYS A 612      23.308  34.819  41.989  1.00 53.34      A
ATOM   4619  CA  LYS A 612      24.483  35.659  41.795  1.00 53.34      A
ATOM   4620  CB  LYS A 612      24.577  36.722  42.892  1.00 78.75      A
ATOM   4621  CG  LYS A 612      25.861  37.546  42.843  1.00 78.75      A
ATOM   4622  CD  LYS A 612      25.649  38.945  43.400  1.00 78.75      A
ATOM   4623  CE  LYS A 612      25.001  38.928  44.776  1.00 78.75      A
ATOM   4624  NZ  LYS A 612      25.831  38.201  45.778  1.00 78.75      A
ATOM   4625  C   LYS A 612      25.709  34.757  41.820  1.00 53.34      A
ATOM   4626  O   LYS A 612      26.601  34.888  40.987  1.00 53.34      A
ATOM   4627  N   GLU A 613      25.751  33.828  42.770  1.00 65.13      A
ATOM   4628  CA  GLU A 613      26.876  32.905  42.833  1.00 65.13      A
ATOM   4629  CB  GLU A 613      26.699  31.901  43.971  1.00101.27      A
ATOM   4630  CG  GLU A 613      27.889  30.965  44.133  1.00101.27      A
ATOM   4631  CD  GLU A 613      27.619  29.829  45.098  1.00101.27      A
ATOM   4632  OE1 GLU A 613      26.792  28.952  44.771  1.00101.27      A
ATOM   4633  OE2 GLU A 613      28.233  29.812  46.184  1.00101.27      A
ATOM   4634  C   GLU A 613      26.944  32.156  41.503  1.00 65.13      A
ATOM   4635  O   GLU A 613      28.019  31.738  41.073  1.00 65.13      A

ATOM   4636  N   PHE A 614      25.788  31.986  40.855  1.00 53.55      A
ATOM   4637  CA  PHE A 614      25.733  31.292  39.573  1.00 53.55      A
ATOM   4638  CB  PHE A 614      24.434  30.486  39.446  1.00 68.97      A
ATOM   4639  CG  PHE A 614      24.501  29.118  40.065  1.00 68.97      A
ATOM   4640  CD1 PHE A 614      23.759  28.068  39.531  1.00 68.97      A
ATOM   4641  CD2 PHE A 614      25.297  28.876  41.182  1.00 68.97      A
ATOM   4642  CE1 PHE A 614      23.810  26.793  40.102  1.00 68.97      A
ATOM   4643  CE2 PHE A 614      25.356  27.606  41.761  1.00 68.97      A
ATOM   4644  CZ  PHE A 614      24.612  26.563  41.221  1.00 68.97      A
ATOM   4645  C   PHE A 614      25.889  32.201  38.352  1.00 53.55      A
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FIGURE 25 CON'T

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ATOM   4646  O   PHE A 614      25.631  31.769  37.224  1.00 53.55      A
ATOM   4647  N   ASN A 615      26.301  33.453  38.584  1.00 55.93      A
ATOM   4648  CA  ASN A 615      26.546  34.437  37.518  1.00 55.93      A
ATOM   4649  CB  ASN A 615      27.310  33.784  36.361  1.00101.28      A
ATOM   4650  CG  ASN A 615      28.714  33.380  36.749  1.00101.28      A
ATOM   4651  OD1 ASN A 615      29.534  34.221  37.117  1.00101.28      A
ATOM   4652  ND2 ASN A 615      29.001  32.084  36.672  1.00101.28      A
ATOM   4653  C   ASN A 615      25.349  35.199  36.950  1.00 55.93      A
ATOM   4654  O   ASN A 615      25.380  35.645  35.803  1.00 55.93      A
ATOM   4655  N   ILE A 616      24.306  35.365  37.752  1.00 50.52      A
ATOM   4656  CA  ILE A 616      23.120  36.088  37.313  1.00 50.52      A
ATOM   4657  CB  ILE A 616      21.991  35.115  36.873  1.00 47.84      A
ATOM   4658  CG2 ILE A 616      20.667  35.856  36.797  1.00 47.84      A
ATOM   4659  CG1 ILE A 616      22.333  34.476  35.527  1.00 47.84      A
ATOM   4660  CD1 ILE A 616      22.217  35.411  34.334  1.00 47.84      A
ATOM   4661  C   ILE A 616      22.596  36.955  38.450  1.00 50.52      A
ATOM   4662  O   ILE A 616      22.113  36.444  39.461  1.00 50.52      A
ATOM   4663  N   LYS A 617      22.690  38.268  38.281  1.00 52.27      A
ATOM   4664  CA  LYS A 617      22.207  39.197  39.298  1.00 52.27      A
ATOM   4665  CB  LYS A 617      23.088  40.446  39.351  1.00 72.78      A
ATOM   4666  CG  LYS A 617      24.537  40.152  39.673  1.00 72.78      A
ATOM   4667  CD  LYS A 617      25.337  41.431  39.836  1.00 72.78      A
ATOM   4668  CE  LYS A 617      26.793  41.122  40.127  1.00 72.78      A
ATOM   4669  NZ  LYS A 617      27.532  42.345  40.532  1.00 72.78      A
ATOM   4670  C   LYS A 617      20.780  39.590  38.960  1.00 52.27      A
ATOM   4671  O   LYS A 617      20.507  40.061  37.851  1.00 52.27      A
ATOM   4672  N   LEU A 618      19.876  39.394  39.915  1.00 66.85      A
ATOM   4673  CA  LEU A 618      18.468  39.711  39.719  1.00 66.85      A
ATOM   4674  CB  LEU A 618      17.592  38.782  40.565  1.00 47.81      A
ATOM   4675  CG  LEU A 618      17.528  37.314  40.129  1.00 47.81      A
ATOM   4676  CD1 LEU A 618      16.642  36.525  41.082  1.00 47.81      A
ATOM   4677  CD2 LEU A 618      16.992  37.240  38.712  1.00 47.81      A
ATOM   4678  C   LEU A 618      18.109  41.159  40.040  1.00 66.85      A
ATOM   4679  O   LEU A 618      17.276  41.765  39.355  1.00 66.85      A
ATOM   4680  N   ASP A 619      18.727  41.709  41.080  1.00100.67      A
ATOM   4681  CA  ASP A 619      18.438  43.079  41.480  1.00100.67      A
ATOM   4682  CB  ASP A 619      19.350  43.504  42.640  1.00105.68      A
ATOM   4683  CG  ASP A 619      20.817  43.366  42.322  1.00105.68      A
ATOM   4684  OD1 ASP A 619      21.225  42.301  41.815  1.00105.68      A
ATOM   4685  OD2 ASP A 619      21.565  44.325  42.600  1.00105.68      A
ATOM   4686  C   ASP A 619      18.546  44.053  40.313  1.00100.67      A
ATOM   4687  O   ASP A 619      19.528  44.045  39.575  1.00100.67      A
ATOM   4688  N   ASN A 620      17.500  44.866  40.158  1.00 62.07      A
ATOM   4689  CA  ASN A 620      17.363  45.876  39.106  1.00 62.07      A
ATOM   4690  CB  ASN A 620      18.731  46.458  38.718  1.00162.12      A
ATOM   4691  CG  ASN A 620      19.295  45.848  37.444  1.00162.12      A
ATOM   4692  OD1 ASN A 620      19.428  44.629  37.326  1.00162.12      A
ATOM   4693  ND2 ASN A 620      19.635  46.700  36.483  1.00162.12      A
ATOM   4694  C   ASN A 620      16.676  45.297  37.866  1.00 62.07      A
ATOM   4695  O   ASN A 620      16.662  45.919  36.797  1.00 62.07      A
ATOM   4696  N   LYS A 621      16.093  44.111  38.011  1.00 50.06      A
ATOM   4697  CA  LYS A 621      15.437  43.459  36.882  1.00 50.06      A
ATOM   4698  CB  LYS A 621      16.150  42.139  36.561  1.00 73.33      A
ATOM   4699  CG  LYS A 621      17.613  42.287  36.174  1.00 73.33      A
ATOM   4700  CD  LYS A 621      17.766  43.143  34.930  1.00 73.33      A
ATOM   4701  CE  LYS A 621      19.204  43.184  34.439  1.00 73.33      A
ATOM   4702  NZ  LYS A 621      19.649  41.849  33.963  1.00 73.33      A
```

FIGURE 25 CON'T

ATOM	4703	C	LYS	A	621	13.946	43.195	37.078	1.00	50.06	A
ATOM	4704	O	LYS	A	521	13.397	43.347	38.175	1.00	50.06	A
ATOM	4705	N	LYS	A	622	13.295	42.817	35.985	1.00	42.86	A
ATOM	4706	CA	LYS	A	622	11.876	42.505	36.006	1.00	42.86	A
ATOM	4707	CB	LYS	A	622	11.144	43.230	34.874	1.00	63.93	A
ATOM	4708	CG	LYS	A	622	9.641	43.076	34.944	1.00	63.93	A
ATOM	4709	CD	LYS	A	622	8.949	43.636	33.708	1.00	63.93	A
ATOM	4710	CE	LYS	A	622	7.442	43.438	33.811	1.00	63.93	A
ATOM	4711	NZ	LYS	A	622	6.714	43.798	32.561	1.00	63.93	A
ATOM	4712	C	LYS	A	622	11.738	40.992	35.833	1.00	42.86	A
ATOM	4713	O	LYS	A	622	12.228	40.419	34.849	1.00	42.86	A
ATOM	4714	N	ILE	A	623	11.088	40.351	36.799	1.00	45.44	A
ATOM	4715	CA	ILE	A	623	10.904	38.909	36.745	1.00	45.44	A
ATOM	4716	CB	ILE	A	623	11.811	38.180	37.765	1.00	48.09	A
ATOM	4717	CG2	ILE	A	623	13.272	38.577	37.555	1.00	48.09	A
ATOM	4718	CG1	ILE	A	623	11.369	38.531	39.187	1.00	48.09	A
ATOM	4719	CD1	ILE	A	623	12.147	37.821	40.266	1.00	48.09	A
ATOM	4720	C	ILE	A	623	9.475	38.469	37.036	1.00	45.44	A
ATOM	4721	O	ILE	A	623	8.725	39.143	37.746	1.00	45.44	A
ATOM	4722	N	LEU	A	624	9.124	37.322	36.463	1.00	46.63	A
ATOM	4723	CA	LEU	A	624	7.833	36.686	36.668	1.00	46.63	A
ATOM	4724	CB	LEU	A	624	7.298	36.129	35.351	1.00	41.36	A
ATOM	4725	CG	LEU	A	624	6.007	35.314	35.418	1.00	41.36	A
ATOM	4726	CD1	LEU	A	624	4.880	36.147	36.026	1.00	41.36	A
ATOM	4727	CD2	LEU	A	624	5.637	34.865	34.004	1.00	41.36	A
ATOM	4728	C	LEU	A	624	8.207	35.534	37.594	1.00	46.63	A
ATOM	4729	O	LEU	A	624	9.013	34.676	37.226	1.00	46.63	A
ATOM	4730	N	LEU	A	625	7.664	35.526	38.803	1.00	44.26	A
ATOM	4731	CA	LEU	A	625	7.989	34.458	39.734	1.00	44.26	A
ATOM	4732	CB	LEU	A	625	8.459	35.022	41.081	1.00	50.85	A
ATOM	4733	CG	LEU	A	625	9.043	33.954	42.015	1.00	50.85	A
ATOM	4734	CD1	LEU	A	625	10.317	34.478	42.652	1.00	50.85	A
ATOM	4735	CD2	LEU	A	625	8.019	33.550	43.066	1.00	50.85	A
ATOM	4736	C	LEU	A	625	6.742	33.634	39.918	1.00	44.26	A
ATOM	4737	O	LEU	A	625	5.671	34.181	40.157	1.00	44.26	A
ATOM	4738	N	LEU	A	626	6.891	32.320	39.808	1.00	40.96	A
ATOM	4739	CA	LEU	A	626	5.764	31.397	39.924	1.00	40.96	A
ATOM	4740	CB	LEU	A	626	5.357	30.906	38.530	1.00	38.76	A
ATOM	4741	CG	LEU	A	626	5.013	31.974	37.479	1.00	38.76	A
ATOM	4742	CD1	LEU	A	626	4.713	31.322	36.134	1.00	38.76	A
ATOM	4743	CD2	LEU	A	626	3.813	32.783	37.967	1.00	38.76	A
ATOM	4744	C	LEU	A	626	6.080	30.188	40.793	1.00	40.96	A
ATOM	4745	O	LEU	A	626	7.239	29.781	40.927	1.00	40.96	A
ATOM	4746	N	ARG	A	627	5.033	29.606	41.361	1.00	44.05	A
ATOM	4747	CA	ARG	A	627	5.158	28.424	42.203	1.00	44.05	A
ATOM	4748	CB	ARG	A	627	5.131	28.834	43.680	1.00	58.33	A
ATOM	4749	CG	ARG	A	627	3.786	29.349	44.165	1.00	58.33	A
ATOM	4750	CD	ARG	A	627	3.082	28.296	45.012	1.00	58.33	A
ATOM	4751	NE	ARG	A	627	3.619	28.237	46.371	1.00	58.33	A
ATOM	4752	CZ	ARG	A	627	3.726	27.125	47.098	1.00	58.33	A
ATOM	4753	NH1	ARG	A	627	3.341	25.951	46.602	1.00	58.33	A
ATOM	4754	NH2	ARG	A	627	4.206	27.189	48.336	1.00	58.33	A
ATOM	4755	C	ARG	A	627	3.978	27.494	41.884	1.00	44.05	A
ATOM	4756	O	ARG	A	627	3.058	27.882	41.162	1.00	44.05	A
ATOM	4757	N	ASP	A	628	4.020	26.270	42.401	1.00	44.99	A
ATOM	4758	CA	ASP	A	628	2.945	25.302	42.193	1.00	44.99	A
ATOM	4759	CB	ASP	A	628	3.445	23.876	42.469	1.00	51.65	A

FIGURE 25 CON'T

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ATOM   4760  CG  ASP A 628       2.382  22.799  42.193  1.00 51.65      A
ATOM   4761  OD1 ASP A 628       1.169  23.090  42.242  1.00 51.65      A
ATOM   4762  OD2 ASP A 628       2.771  21.642  41.941  1.00 51.65      A
ATOM   4763  C   ASP A 628       1.817  25.628  43.167  1.00 44.99      A

ATOM   4764  O   ASP A 628       1.857  25.212  44.325  1.00 44.99      A
ATOM   4765  N   GLY A 629       0.817  26.370  42.703  1.00 45.09      A
ATOM   4766  CA  GLY A 629      -0.297  26.705  43.566  1.00 45.09      A
ATOM   4767  C   GLY A 629      -0.450  28.184  43.880  1.00 45.09      A
ATOM   4768  O   GLY A 629       0.061  29.051  43.157  1.00 45.09      A
ATOM   4769  N   ARG A 630      -1.142  28.471  44.976  1.00 58.81      A
ATOM   4770  CA  ARG A 630      -1.384  29.845  45.380  1.00 58.81      A
ATOM   4771  CB  ARG A 630      -2.609  29.902  46.298  1.00105.79      A
ATOM   4772  CG  ARG A 630      -3.080  31.311  46.619  1.00105.79      A
ATOM   4773  CD  ARG A 630      -4.225  31.306  47.619  1.00105.79      A
ATOM   4774  NE  ARG A 630      -3.816  30.714  48.888  1.00105.79      A
ATOM   4775  CZ  ARG A 630      -4.628  30.520  49.921  1.00105.79      A
ATOM   4776  NH1 ARG A 630      -5.904  30.872  49.842  1.00105.79      A
ATOM   4777  NH2 ARG A 630      -4.163  29.966  51.033  1.00105.79      A
ATOM   4778  C   ARG A 630      -0.184  30.486  46.077  1.00 58.81      A
ATOM   4779  O   ARG A 630       0.557  29.825  46.803  1.00 58.81      A
ATOM   4780  N   ILE A 631       0.012  31.777  45.827  1.00 52.71      A
ATOM   4781  CA  ILE A 631       1.086  32.532  46.464  1.00 52.71      A
ATOM   4782  CB  ILE A 631       1.327  33.881  45.748  1.00 62.65      A
ATOM   4783  CG2 ILE A 631       2.466  34.640  46.426  1.00 62.65      A
ATOM   4784  CG1 ILE A 631       1.612  33.644  44.261  1.00 62.65      A
ATOM   4785  CD1 ILE A 631       2.805  32.762  43.995  1.00 62.65      A
ATOM   4786  C   ILE A 631       0.605  32.827  47.889  1.00 52.71      A
ATOM   4787  O   ILE A 631      -0.390  33.516  48.071  1.00 52.71      A
ATOM   4788  N   THR A 632       1.304  32.308  48.893  1.00 47.14      A
ATOM   4789  CA  THR A 632       0.914  32.533  50.288  1.00 47.14      A
ATOM   4790  CB  THR A 632       1.645  31.563  51.237  1.00 53.31      A
ATOM   4791  OG1 THR A 632       3.047  31.864  51.221  1.00 53.31      A
ATOM   4792  CG2 THR A 632       1.433  30.108  50.807  1.00 53.31      A
ATOM   4793  C   THR A 632       1.248  33.959  50.753  1.00 47.14      A
ATOM   4794  O   THR A 632       2.007  34.685  50.097  1.00 47.14      A
ATOM   4795  N   ASN A 633       0.686  34.344  51.896  1.00 59.80      A
ATOM   4796  CA  ASN A 633       0.940  35.666  52.455  1.00 59.80      A
ATOM   4797  CB  ASN A 633       0.122  35.877  53.731  1.00 86.65      A
ATOM   4798  CG  ASN A 633      -1.370  35.813  53.480  1.00 86.65      A
ATOM   4799  OD1 ASN A 633      -1.874  36.395  52.517  1.00 86.65      A
ATOM   4800  ND2 ASN A 633      -2.089  35.111  54.350  1.00 86.65      A
ATOM   4801  C   ASN A 633       2.424  35.794  52.762  1.00 59.80      A
ATOM   4802  O   ASN A 633       3.041  36.825  52.479  1.00 59.80      A
ATOM   4803  N   ASN A 634       2.992  34.736  53.334  1.00 51.78      A
ATOM   4804  CA  ASN A 634       4.410  34.717  53.669  1.00 51.78      A
ATOM   4805  CB  ASN A 634       4.762  33.434  54.432  1.00 64.55      A
ATOM   4806  CG  ASN A 634       4.318  33.478  55.886  1.00 64.55      A
ATOM   4807  OD1 ASN A 634       3.706  34.453  56.335  1.00 64.55      A
ATOM   4808  ND2 ASN A 634       4.628  32.421  56.629  1.00 64.55      A
ATOM   4809  C   ASN A 634       5.277  34.821  52.423  1.00 51.78      A
ATOM   4810  O   ASN A 634       6.350  35.432  52.455  1.00 51.78      A
ATOM   4811  N   GLU A 635       4.828  34.224  51.322  1.00 53.86      A
ATOM   4812  CA  GLU A 635       5.606  34.292  50.093  1.00 53.86      A
ATOM   4813  CB  GLU A 635       5.140  33.226  49.098  1.00 57.25      A
ATOM   4814  CG  GLU A 635       5.447  31.815  49.584  1.00 57.25      A
ATOM   4815  CD  GLU A 635       4.832  30.732  48.720  1.00 57.25      A
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FIGURE 25 CON'T

ATOM	4816	OE1	GLU	A	635	3.652	30.872	48.345	1.00	57.25	A
ATOM	4817	OE2	GLU	A	635	5.527	29.736	48.429	1.00	57.25	A
ATOM	4818	C	GLU	A	635	5.513	35.685	49.498	1.00	53.86	A
ATOM	4819	O	GLU	A	635	6.471	36.174	48.900	1.00	53.86	A
ATOM	4820	N	GLU	A	636	4.371	36.335	49.678	1.00	53.88	A
ATOM	4821	CA	GLU	A	636	4.216	37.688	49.169	1.00	53.88	A
ATOM	4822	CB	GLU	A	636	2.764	38.154	49.296	1.00	73.18	A
ATOM	4823	CG	GLU	A	636	2.536	39.571	48.792	1.00	73.18	A
ATOM	4824	CD	GLU	A	636	1.073	39.954	48.759	1.00	73.18	A
ATOM	4825	OE1	GLU	A	636	0.340	39.440	47.890	1.00	73.18	A
ATOM	4826	OE2	GLU	A	636	0.656	40.768	49.607	1.00	73.18	A
ATOM	4827	C	GLU	A	636	5.142	38.603	49.979	1.00	53.88	A
ATOM	4828	O	GLU	A	636	5.880	39.414	49.412	1.00	53.88	A
ATOM	4829	N	GLU	A	637	5.116	38.458	51.301	1.00	60.42	A
ATOM	4830	CA	GLU	A	637	5.978	39.263	52.165	1.00	60.42	A
ATOM	4831	CB	GLU	A	637	5.847	38.838	53.630	1.00	135.81	A
ATOM	4832	CG	GLU	A	637	4.536	39.200	54.291	1.00	135.81	A
ATOM	4833	CD	GLU	A	637	4.569	38.962	55.788	1.00	135.81	A
ATOM	4834	OE1	GLU	A	637	4.805	37.807	56.200	1.00	135.81	A
ATOM	4835	OE2	GLU	A	637	4.365	39.930	56.551	1.00	135.81	A
ATOM	4836	C	GLU	A	637	7.416	39.057	51.729	1.00	60.42	A
ATOM	4837	O	GLU	A	637	8.153	40.015	51.471	1.00	60.42	A
ATOM	4838	N	GLY	A	638	7.804	37.786	51.656	1.00	47.17	A
ATOM	4839	CA	GLY	A	638	9.149	37.443	51.250	1.00	47.17	A
ATOM	4840	C	GLY	A	638	9.479	38.087	49.927	1.00	47.17	A
ATOM	4841	O	GLY	A	638	10.621	38.474	49.697	1.00	47.17	A
ATOM	4842	N	LEU	A	639	8.487	38.204	49.050	1.00	49.32	A
ATOM	4843	CA	LEU	A	639	8.719	38.819	47.744	1.00	49.32	A
ATOM	4844	CB	LEU	A	639	7.638	38.387	46.749	1.00	56.98	A
ATOM	4845	CG	LEU	A	639	7.688	36.923	46.308	1.00	56.98	A
ATOM	4846	CD1	LEU	A	639	6.629	36.690	45.251	1.00	56.98	A
ATOM	4847	CD2	LEU	A	639	9.060	36.595	45.743	1.00	56.98	A
ATOM	4848	C	LEU	A	639	8.786	40.351	47.833	1.00	49.32	A
ATOM	4849	O	LEU	A	639	9.463	40.999	47.029	1.00	49.32	A
ATOM	4850	N	LYS	A	640	8.079	40.933	48.795	1.00	68.00	A
ATOM	4851	CA	LYS	A	640	8.131	42.379	48.966	1.00	68.00	A
ATOM	4852	CB	LYS	A	640	7.088	42.850	49.991	1.00	63.26	A
ATOM	4853	CG	LYS	A	640	5.640	42.686	49.529	1.00	63.26	A
ATOM	4854	CD	LYS	A	640	4.654	43.472	50.402	1.00	63.26	A
ATOM	4855	CE	LYS	A	640	4.583	42.949	51.832	1.00	63.26	A
ATOM	4856	NZ	LYS	A	640	3.587	43.707	52.654	1.00	63.26	A
ATOM	4857	C	LYS	A	640	9.541	42.683	49.472	1.00	68.00	A
ATOM	4858	O	LYS	A	640	10.181	43.653	49.059	1.00	68.00	A
ATOM	4859	N	TYR	A	641	10.019	41.810	50.354	1.00	68.42	A
ATOM	4860	CA	TYR	A	641	11.339	41.917	50.961	1.00	68.42	A
ATOM	4861	CB	TYR	A	641	11.549	40.711	51.874	1.00	67.22	A
ATOM	4862	CG	TYR	A	641	12.853	40.700	52.630	1.00	67.22	A
ATOM	4863	CD1	TYR	A	641	13.122	41.659	53.608	1.00	67.22	A
ATOM	4864	CE1	TYR	A	641	14.312	41.625	54.339	1.00	67.22	A
ATOM	4865	CD2	TYR	A	641	13.806	39.710	52.393	1.00	67.22	A
ATOM	4866	CE2	TYR	A	641	14.994	39.667	53.111	1.00	67.22	A
ATOM	4867	CZ	TYR	A	641	15.243	40.625	54.085	1.00	67.22	A
ATOM	4868	OH	TYR	A	641	16.416	40.580	54.806	1.00	67.22	A
ATOM	4869	C	TYR	A	641	12.453	41.983	49.912	1.00	68.42	A
ATOM	4870	O	TYR	A	641	13.265	42.906	49.897	1.00	68.42	A
ATOM	4871	N	ILE	A	642	12.475	40.985	49.038	1.00	56.35	A
ATOM	4872	CA	ILE	A	642	13.462	40.872	47.970	1.00	56.35	A

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ATOM   4873  CB  ILE A 642      13.351  39.460  47.329  1.00 86.15      A
ATOM   4874  CG2 ILE A 642      11.907  39.184  46.934  1.00 86.15      A
ATOM   4875  CG1 ILE A 642      14.264  39.330  46.116  1.00 86.15      A
ATOM   4876  CD1 ILE A 642      14.002  38.056  45.315  1.00 86.15      A
ATOM   4877  C   ILE A 642      13.278  41.967  46.905  1.00 56.35      A
ATOM   4878  O   ILE A 642      14.208  42.301  46.173  1.00 56.35      A
ATOM   4879  N   SER A 643      12.076  42.523  46.822  1.00 60.93      A
ATOM   4880  CA  SER A 643      11.786  43.572  45.846  1.00 60.93      A
ATOM   4881  CB  SER A 643      10.271  43.761  45.710  1.00 54.02      A
ATOM   4882  OG  SER A 643       9.945  44.827  44.830  1.00 54.02      A
ATOM   4883  C   SER A 643      12.432  44.893  46.256  1.00 60.93      A
ATOM   4884  O   SER A 643      13.083  45.553  45.444  1.00 60.93      A
ATOM   4885  N   GLU A 644      12.245  45.273  47.516  1.00 75.63      A
ATOM   4886  CA  GLU A 644      12.814  46.515  48.021  1.00 75.63      A
ATOM   4887  CB  GLU A 644      12.196  46.870  49.378  1.00159.47      A
ATOM   4888  CG  GLU A 644      12.866  48.046  50.082  1.00159.47      A
ATOM   4889  CD  GLU A 644      12.995  49.271  49.192  1.00159.47      A
ATOM   4890  OE1 GLU A 644      11.959  49.782  48.717  1.00159.47      A
ATOM   4891  OE2 GLU A 644      14.138  49.724  48.966  1.00159.47      A

ATOM   4892  C   GLU A 644      14.327  46.413  48.155  1.00 75.63      A
ATOM   4893  O   GLU A 644      15.068  47.231  47.605  1.00 75.63      A
ATOM   4894  N   MSE A 645      14.778  45.394  48.877  1.00 71.24      A
ATOM   4895  CA  MSE A 645      16.199  45.183  49.108  1.00 71.24      A
ATOM   4896  CB  MSE A 645      16.413  43.877  49.880  1.00 69.55      A
ATOM   4897  CG  MSE A 645      17.879  43.527  50.099  1.00 69.55      A
ATOM   4898  SE  MSE A 645      18.158  41.917  51.128  1.00 69.55      A
ATOM   4899  CE  MSE A 645      17.652  42.616  52.856  1.00 69.55      A
ATOM   4900  C   MSE A 645      17.050  45.169  47.840  1.00 71.24      A
ATOM   4901  O   MSE A 645      18.138  45.742  47.813  1.00 71.24      A
ATOM   4902  N   PHE A 646      16.554  44.524  46.789  1.00 51.49      A
ATOM   4903  CA  PHE A 646      17.306  44.414  45.544  1.00 51.49      A
ATOM   4904  CB  PHE A 646      17.384  42.941  45.128  1.00 57.55      A
ATOM   4905  CG  PHE A 646      18.132  42.071  46.096  1.00 57.55      A
ATOM   4906  CD1 PHE A 646      19.519  42.118  46.166  1.00 57.55      A
ATOM   4907  CD2 PHE A 646      17.445  41.210  46.950  1.00 57.55      A
ATOM   4908  CE1 PHE A 646      20.217  41.316  47.078  1.00 57.55      A
ATOM   4909  CE2 PHE A 646      18.126  40.408  47.861  1.00 57.55      A
ATOM   4910  CZ  PHE A 646      19.516  40.459  47.928  1.00 57.55      A
ATOM   4911  C   PHE A 646      16.734  45.218  44.386  1.00 51.49      A
ATOM   4912  O   PHE A 646      17.254  45.147  43.273  1.00 51.49      A
ATOM   4913  N   ASP A 647      15.673  45.981  44.633  1.00 57.02      A
ATOM   4914  CA  ASP A 647      15.039  46.755  43.562  1.00 57.02      A
ATOM   4915  CB  ASP A 647      15.992  47.828  43.012  1.00 72.79      A
ATOM   4916  CG  ASP A 647      16.262  48.941  44.010  1.00 72.79      A
ATOM   4917  OD1 ASP A 647      15.288  49.563  44.489  1.00 72.79      A
ATOM   4918  OD2 ASP A 647      17.447  49.196  44.310  1.00 72.79      A
ATOM   4919  C   ASP A 647      14.615  45.811  42.429  1.00 57.02      A
ATOM   4920  O   ASP A 647      14.929  46.026  41.254  1.00 57.02      A
ATOM   4921  N   ILE A 648      13.917  44.747  42.798  1.00 55.16      A
ATOM   4922  CA  ILE A 648      13.443  43.783  41.816  1.00 55.16      A
ATOM   4923  CB  ILE A 648      13.634  42.323  42.324  1.00 54.96      A
ATOM   4924  CG2 ILE A 648      13.066  41.326  41.302  1.00 54.96      A
ATOM   4925  CG1 ILE A 648      15.122  42.050  42.573  1.00 54.96      A
ATOM   4926  CD1 ILE A 648      15.404  40.717  43.254  1.00 54.96      A
ATOM   4927  C   ILE A 648      11.961  44.035  41.586  1.00 55.16      A
ATOM   4928  O   ILE A 648      11.195  44.126  42.542  1.00 55.16      A
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FIGURE 25 CON'T

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ATOM   4929  N   GLU A 649      11.562  44.184  40.328  1.00 43.65      A
ATOM   4930  CA  GLU A 649      10.147  44.379  40.013  1.00 43.65      A
ATOM   4931  CB  GLU A 649       9.971  45.137  38.696  1.00 74.80      A
ATOM   4932  CG  GLU A 649       8.520  45.475  38.389  1.00 74.80      A
ATOM   4933  CD  GLU A 649       8.316  46.079  37.006  1.00 74.80      A
ATOM   4934  OE1 GLU A 649       7.149  46.344  36.648  1.00 74.80      A
ATOM   4935  OE2 GLU A 649       9.309  46.290  36.275  1.00 74.80      A
ATOM   4936  C   GLU A 649       9.593  42.956  39.875  1.00 43.65      A
ATOM   4937  O   GLU A 649       9.868  42.270  38.889  1.00 43.65      A
ATOM   4938  N   VAL A 650       8.825  42.515  40.869  1.00 51.93      A
ATOM   4939  CA  VAL A 650       8.281  41.158  40.868  1.00 51.93      A
ATOM   4940  CB  VAL A 650       8.378  40.504  42.277  1.00 53.47      A
ATOM   4941  CG1 VAL A 650       8.045  39.018  42.181  1.00 53.47      A
ATOM   4942  CG2 VAL A 650       9.761  40.719  42.877  1.00 53.47      A
ATOM   4943  C   VAL A 650       6.833  40.997  40.440  1.00 51.93      A
ATOM   4944  O   VAL A 650       5.938  41.537  41.073  1.00 51.93      A
ATOM   4945  N   VAL A 651       6.605  40.239  39.372  1.00 46.48      A
ATOM   4946  CA  VAL A 651       5.244  39.955  38.927  1.00 46.48      A
ATOM   4947  CB  VAL A 651       5.070  40.116  37.398  1.00 47.71      A
ATOM   4948  CG1 VAL A 651       3.640  39.765  36.999  1.00 47.71      A
ATOM   4949  CG2 VAL A 651       5.388  41.537  36.978  1.00 47.71      A
ATOM   4950  C   VAL A 651       4.968  38.491  39.300  1.00 46.48      A
ATOM   4951  O   VAL A 651       5.795  37.603  39.046  1.00 46.48      A
ATOM   4952  N   THR A 652       3.818  38.240  39.916  1.00 49.59      A
ATOM   4953  CA  THR A 652       3.474  36.884  40.309  1.00 49.59      A
ATOM   4954  CB  THR A 652       4.056  36.552  41.709  1.00 46.75      A
ATOM   4955  OG1 THR A 652       3.934  35.145  41.959  1.00 46.75      A
ATOM   4956  CG2 THR A 652       3.314  37.319  42.798  1.00 46.75      A
ATOM   4957  C   THR A 652       1.967  36.691  40.317  1.00 49.59      A
ATOM   4958  O   THR A 652       1.214  37.661  40.237  1.00 49.59      A
ATOM   4959  N   MSE A 653       1.537  35.435  40.409  1.00 46.98      A
ATOM   4960  CA  MSE A 653       0.116  35.087  40.432  1.00 46.98      A
ATOM   4961  CB  MSE A 653      -0.491  35.262  39.035  1.00 57.38      A
ATOM   4962  CG  MSE A 653      -0.007  34.233  38.043  1.00 57.38      A
ATOM   4963  SE  MSE A 653      -0.624  34.530  36.245  1.00 57.38      A
ATOM   4964  CE  MSE A 653       0.932  35.480  35.569  1.00 57.38      A
ATOM   4965  C   MSE A 653      -0.077  33.630  40.871  1.00 46.98      A
ATOM   4966  O   MSE A 653       0.872  32.851  40.901  1.00 46.98      A
ATOM   4967  N   ASP A 654      -1.308  33.269  41.213  1.00 51.12      A
ATOM   4968  CA  ASP A 654      -1.613  31.897  41.607  1.00 51.12      A
ATOM   4969  CB  ASP A 654      -2.954  31.814  42.348  1.00 53.20      A
ATOM   4970  CG  ASP A 654      -2.953  32.565  43.673  1.00 53.20      A
ATOM   4971  OD1 ASP A 654      -1.868  32.770  44.272  1.00 53.20      A
ATOM   4972  OD2 ASP A 654      -4.060  32.930  44.128  1.00 53.20      A
ATOM   4973  C   ASP A 654      -1.709  31.022  40.354  1.00 51.12      A
ATOM   4974  O   ASP A 654      -2.436  31.355  39.416  1.00 51.12      A
ATOM   4975  N   VAL A 655      -0.964  29.918  40.335  1.00 44.06      A
ATOM   4976  CA  VAL A 655      -1.004  28.980  39.223  1.00 44.06      A
ATOM   4977  CB  VAL A 655       0.377  28.790  38.589  1.00 43.58      A
ATOM   4978  CG1 VAL A 655       0.286  27.774  37.468  1.00 43.58      A
ATOM   4979  CG2 VAL A 655       0.884  30.112  38.057  1.00 43.58      A
ATOM   4980  C   VAL A 655      -1.475  27.681  39.863  1.00 44.06      A
ATOM   4981  O   VAL A 655      -0.692  26.930  40.457  1.00 44.06      A
ATOM   4982  N   ILE A 656      -2.772  27.428  39.740  1.00 46.88      A
ATOM   4983  CA  ILE A 656      -3.392  26.276  40.368  1.00 46.88      A
ATOM   4984  CB  ILE A 656      -4.638  26.756  41.150  1.00 39.39      A
ATOM   4985  CG2 ILE A 656      -5.289  25.599  41.887  1.00 39.39      A
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FIGURE 25 CON'T

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ATOM   4986  CG1 ILE A 656      -4.222  27.850  42.137  1.00 39.39      A
ATOM   4987  CD1 ILE A 656      -5.385  28.702  42.646  1.00 39.39      A
ATOM   4988  C   ILE A 656      -3.766  25.140  39.420  1.00 46.88      A
ATOM   4989  O   ILE A 656      -4.572  25.310  38.498  1.00 46.88      A
ATOM   4990  N   LYS A 657      -3.176  23.976  39.665  1.00 42.94      A
ATOM   4991  CA  LYS A 657      -3.442  22.805  38.848  1.00 42.94      A
ATOM   4992  CB  LYS A 657      -2.150  22.009  38.604  1.00 49.37      A
ATOM   4993  CG  LYS A 657      -1.608  21.245  39.811  1.00 49.37      A
ATOM   4994  CD  LYS A 657      -0.314  20.513  39.435  1.00 49.37      A
ATOM   4995  CE  LYS A 657       0.054  19.413  40.436  1.00 49.37      A
ATOM   4996  NZ  LYS A 657       0.180  19.904  41.836  1.00 49.37      A
ATOM   4997  C   LYS A 657      -4.482  21.920  39.536  1.00 42.94      A
ATOM   4998  O   LYS A 657      -5.128  21.103  38.891  1.00 42.94      A
ATOM   4999  N   ASN A 658      -4.645  22.094  40.843  1.00 43.70      A
ATOM   5000  CA  ASN A 658      -5.600  21.295  41.594  1.00 43.70      A
ATOM   5001  CB  ASN A 658      -4.952  20.728  42.864  1.00 76.60      A
ATOM   5002  CG  ASN A 658      -3.824  19.754  42.560  1.00 76.60      A
ATOM   5003  OD1 ASN A 658      -3.961  18.871  41.711  1.00 76.60      A
ATOM   5004  ND2 ASN A 658      -2.705  19.907  43.262  1.00 76.60      A
ATOM   5005  C   ASN A 658      -6.833  22.089  41.962  1.00 43.70      A
ATOM   5006  O   ASN A 658      -6.875  22.780  42.974  1.00 43.70      A
ATOM   5007  N   HIS A 659      -7.844  21.977  41.118  1.00 37.49      A
ATOM   5008  CA  HIS A 659      -9.100  22.672  41.312  1.00 37.49      A
ATOM   5009  CB  HIS A 659      -9.046  24.038  40.602  1.00 35.90      A
ATOM   5010  CG  HIS A 659      -8.790  23.944  39.130  1.00 35.90      A
ATOM   5011  CD2 HIS A 659      -7.631  23.935  38.424  1.00 35.90      A
ATOM   5012  ND1 HIS A 659      -9.798  23.722  38.213  1.00 35.90      A
ATOM   5013  CE1 HIS A 659      -9.270  23.574  37.010  1.00 35.90      A
ATOM   5014  NE2 HIS A 659      -7.957  23.699  37.109  1.00 35.90      A
ATOM   5015  C   HIS A 659     -10.110  21.710  40.691  1.00 37.49      A
ATOM   5016  O   HIS A 659      -9.733  20.806  39.936  1.00 37.49      A
ATOM   5017  N   PRO A 660     -11.401  21.890  40.997  1.00 33.96      A
ATOM   5018  CD  PRO A 660     -11.929  22.848  41.994  1.00 33.10      A
ATOM   5019  CA  PRO A 660     -12.467  21.031  40.489  1.00 33.96      A
                                .
ATOM   5020  CB  PRO A 660     -13.427  21.002  41.662  1.00 33.10      A
ATOM   5021  CG  PRO A 660     -13.415  22.494  42.056  1.00 33.10      A
ATOM   5022  C   PRO A 660     -13.190  21.442  39.193  1.00 33.96      A
ATOM   5023  O   PRO A 660     -14.043  20.710  38.719  1.00 33.96      A
ATOM   5024  N   VAL A 661     -12.866  22.601  38.634  1.00 38.34      A
ATOM   5025  CA  VAL A 661     -13.550  23.073  37.435  1.00 38.34      A
ATOM   5026  CB  VAL A 661     -13.310  24.582  37.230  1.00 39.74      A
ATOM   5027  CG1 VAL A 661     -13.938  25.042  35.923  1.00 39.74      A
ATOM   5028  CG2 VAL A 661     -13.908  25.356  38.392  1.00 39.74      A
ATOM   5029  C   VAL A 661     -13.161  22.341  36.164  1.00 38.34      A
ATOM   5030  O   VAL A 661     -11.983  22.202  35.858  1.00 38.34      A
ATOM   5031  N   ARG A 662     -14.155  21.860  35.427  1.00 38.85      A
ATOM   5032  CA  ARG A 662     -13.895  21.147  34.172  1.00 38.85      A
ATOM   5033  CB  ARG A 662     -14.116  19.643  34.365  1.00 38.35      A
ATOM   5034  CG  ARG A 662     -13.129  18.981  35.351  1.00 38.35      A
ATOM   5035  CD  ARG A 662     -11.704  18.956  34.794  1.00 38.35      A
ATOM   5036  NE  ARG A 662     -10.762  18.319  35.712  1.00 38.35      A
ATOM   5037  CZ  ARG A 662     -10.229  18.908  36.782  1.00 38.35      A
ATOM   5038  NH1 ARG A 662     -10.531  20.165  37.080  1.00 38.35      A
ATOM   5039  NH2 ARG A 662      -9.411  18.226  37.567  1.00 38.35      A
ATOM   5040  C   ARG A 662     -14.786  21.652  33.032  1.00 38.85      A
ATOM   5041  O   ARG A 662     -15.963  21.953  33.250  1.00 38.85      A
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FIGURE 25 CON'T

ATOM	5042	N	ALA	A	663	-14.201	21.769	31.839	1.00	45.78	A
ATOM	5043	CA	ALA	A	663	-14.920	22.196	30.628	1.00	45.78	A
ATOM	5044	CB	ALA	A	663	-14.133	23.258	29.870	1.00	44.45	A
ATOM	5045	C	ALA	A	663	-15.030	20.938	29.787	1.00	45.78	A
ATOM	5046	O	ALA	A	663	-14.016	20.307	29.457	1.00	45.78	A
ATOM	5047	N	PHE	A	664	-16.255	20.570	29.441	1.00	48.74	A
ATOM	5048	CA	PHE	A	664	-16.479	19.347	28.685	1.00	48.74	A
ATOM	5049	CB	PHE	A	664	-17.866	18.808	29.022	1.00	42.62	A
ATOM	5050	CG	PHE	A	664	-18.045	18.505	30.480	1.00	42.62	A
ATOM	5051	CD1	PHE	A	664	-17.025	17.870	31.199	1.00	42.62	A
ATOM	5052	CD2	PHE	A	664	-19.224	18.826	31.133	1.00	42.62	A
ATOM	5053	CE1	PHE	A	664	-17.186	17.560	32.550	1.00	42.62	A
ATOM	5054	CE2	PHE	A	664	-19.397	18.520	32.483	1.00	42.62	A
ATOM	5055	CZ	PHE	A	664	-18.372	17.884	33.194	1.00	42.62	A
ATOM	5056	C	PHE	A	664	-16.274	19.402	27.175	1.00	48.74	A
ATOM	5057	O	PHE	A	664	-17.210	19.226	26.390	1.00	48.74	A
ATOM	5058	N	ALA	A	665	-15.027	19.638	26.786	1.00	51.15	A
ATOM	5059	CA	ALA	A	665	-14.627	19.699	25.388	1.00	51.15	A
ATOM	5060	CB	ALA	A	665	-14.886	21.103	24.810	1.00	44.63	A
ATOM	5061	C	ALA	A	665	-13.138	19.391	25.370	1.00	51.15	A
ATOM	5062	O	ALA	A	665	-12.421	19.763	26.296	1.00	51.15	A
ATOM	5063	N	ASN	A	666	-12.671	18.701	24.336	1.00	53.36	A
ATOM	5064	CA	ASN	A	666	-11.253	18.397	24.246	1.00	53.36	A
ATOM	5065	CB	ASN	A	666	-11.030	16.927	23.878	1.00	54.17	A
ATOM	5066	CG	ASN	A	666	-9.549	16.553	23.853	1.00	54.17	A
ATOM	5067	OD1	ASN	A	666	-8.746	17.119	24.593	1.00	54.17	A
ATOM	5068	ND2	ASN	A	666	-9.189	15.589	23.009	1.00	54.17	A
ATOM	5069	C	ASN	A	666	-10.594	19.314	23.221	1.00	53.36	A
ATOM	5070	O	ASN	A	666	-10.374	18.936	22.074	1.00	53.36	A
ATOM	5071	N	MSE	A	667	-10.299	20.536	23.645	1.00	46.65	A
ATOM	5072	CA	MSE	A	667	-9.653	21.513	22.779	1.00	46.65	A
ATOM	5073	CB	MSE	A	667	-10.680	22.187	21.847	1.00	79.72	A
ATOM	5074	CG	MSE	A	667	-11.765	23.012	22.549	1.00	79.72	A
ATOM	5075	SE	MSE	A	667	-12.931	24.041	21.337	1.00	79.72	A
ATOM	5076	CE	MSE	A	667	-12.819	25.765	22.187	1.00	79.72	A
ATOM	5077	C	MSE	A	667	-8.951	22.584	23.606	1.00	46.65	A
ATOM	5078	O	MSE	A	667	-9.263	22.783	24.778	1.00	46.65	A
ATOM	5079	N	LYS	A	668	-8.005	23.269	22.975	1.00	56.56	A
ATOM	5080	CA	LYS	A	668	-7.265	24.341	23.619	1.00	56.56	A
ATOM	5081	CB	LYS	A	668	-6.034	24.702	22.785	1.00	74.88	A
ATOM	5082	CG	LYS	A	668	-5.040	23.556	22.646	1.00	74.88	A
ATOM	5083	CD	LYS	A	668	-3.838	23.949	21.800	1.00	74.88	A
ATOM	5084	CE	LYS	A	668	-4.200	24.077	20.323	1.00	74.88	A
ATOM	5085	NZ	LYS	A	668	-4.605	22.768	19.742	1.00	74.88	A
ATOM	5086	C	LYS	A	668	-8.197	25.536	23.736	1.00	56.56	A
ATOM	5087	O	LYS	A	668	-8.907	25.875	22.788	1.00	56.56	A
ATOM	5088	N	MSE	A	669	-8.183	26.175	24.902	1.00	48.15	A
ATOM	5089	CA	MSE	A	669	-9.049	27.314	25.176	1.00	48.15	A
ATOM	5090	CB	MSE	A	669	-10.495	26.824	25.261	1.00	60.60	A
ATOM	5091	CG	MSE	A	669	-10.694	25.792	26.376	1.00	60.60	A
ATOM	5092	SE	MSE	A	669	-12.469	25.027	26.528	1.00	60.60	A
ATOM	5093	CE	MSE	A	669	-13.075	26.047	27.994	1.00	60.60	A
ATOM	5094	C	MSE	A	669	-8.680	27.962	26.510	1.00	48.15	A
ATOM	5095	O	MSE	A	669	-7.782	27.509	27.210	1.00	48.15	A
ATOM	5096	N	TYR	A	670	-9.394	29.025	26.849	1.00	45.94	A
ATOM	5097	CA	TYR	A	670	-9.225	29.723	28.114	1.00	45.94	A
ATOM	5098	CB	TYR	A	670	-7.957	30.586	28.112	1.00	56.73	A

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ATOM   5099  CG  TYR A 670     -7.970  31.781  27.187  1.00 56.73      A
ATOM   5100  CD1 TYR A 670     -8.536  32.992  27.584  1.00 56.73      A
ATOM   5101  CE1 TYR A 670     -8.507  34.109  26.742  1.00 56.73      A
ATOM   5102  CD2 TYR A 670     -7.381  31.711  25.922  1.00 56.73      A
ATOM   5103  CE2 TYR A 670     -7.349  32.812  25.082  1.00 56.73      A
ATOM   5104  CZ  TYR A 670     -7.911  34.005  25.496  1.00 56.73      A
ATOM   5105  OH  TYR A 670     -7.871  35.093  24.661  1.00 56.73      A
ATOM   5106  C   TYR A 670    -10.482  30.566  28.315  1.00 45.94      A
ATOM   5107  O   TYR A 670    -11.115  30.978  27.345  1.00 45.94      A
ATOM   5108  N   PHE A 671    -10.861  30.802  29.565  1.00 46.51      A
ATOM   5109  CA  PHE A 671    -12.061  31.576  29.847  1.00 46.51      A
ATOM   5110  CB  PHE A 671    -13.313  30.685  29.689  1.00 39.62      A
ATOM   5111  CG  PHE A 671    -13.316  29.452  30.570  1.00 39.62      A
ATOM   5112  CD1 PHE A 671    -13.831  29.495  31.860  1.00 39.62      A
ATOM   5113  CD2 PHE A 671    -12.805  28.246  30.102  1.00 39.62      A
ATOM   5114  CE1 PHE A 671    -13.838  28.340  32.680  1.00 39.62      A
ATOM   5115  CE2 PHE A 671    -12.807  27.089  30.910  1.00 39.62      A
ATOM   5116  CZ  PHE A 671    -13.325  27.143  32.201  1.00 39.62      A
ATOM   5117  C   PHE A 671    -12.011  32.167  31.247  1.00 46.51      A
ATOM   5118  O   PHE A 671    -11.259  31.696  32.105  1.00 46.51      A
ATOM   5119  N   ASN A 672    -12.815  33.200  31.473  1.00 46.97      A
ATOM   5120  CA  ASN A 672    -12.867  33.854  32.771  1.00 46.97      A
ATOM   5121  CB  ASN A 672    -13.041  35.373  32.607  1.00 66.45      A
ATOM   5122  CG  ASN A 672    -13.073  36.119  33.946  1.00 66.45      A
ATOM   5123  OD1 ASN A 672    -13.911  35.847  34.816  1.00 66.45      A
ATOM   5124  ND2 ASN A 672    -12.163  37.073  34.109  1.00 66.45      A
ATOM   5125  C   ASN A 672    -14.048  33.294  33.531  1.00 46.97      A
ATOM   5126  O   ASN A 672    -15.167  33.286  33.027  1.00 46.97      A
ATOM   5127  N   LEU A 673    -13.795  32.803  34.736  1.00 44.10      A
ATOM   5128  CA  LEU A 673    -14.862  32.272  35.560  1.00 44.10      A
ATOM   5129  CB  LEU A 673    -14.924  30.743  35.500  1.00 33.68      A
ATOM   5130  CG  LEU A 673    -15.806  30.104  36.581  1.00 33.68      A
ATOM   5131  CD1 LEU A 673    -17.270  30.492  36.333  1.00 33.68      A
ATOM   5132  CD2 LEU A 673    -15.648  28.595  36.564  1.00 33.68      A
ATOM   5133  C   LEU A 673    -14.591  32.700  36.971  1.00 44.10      A
ATOM   5134  O   LEU A 673    -13.539  32.393  37.526  1.00 44.10      A
ATOM   5135  N   GLY A 674    -15.541  33.426  37.542  1.00 48.61      A
ATOM   5136  CA  GLY A 674    -15.401  33.878  38.908  1.00 48.61      A
ATOM   5137  C   GLY A 674    -14.193  34.749  39.193  1.00 48.61      A
ATOM   5138  O   GLY A 674    -13.755  34.805  40.332  1.00 48.61      A
ATOM   5139  N   GLY A 675    -13.656  35.425  38.184  1.00 53.58      A
ATOM   5140  CA  GLY A 675    -12.504  36.278  38.418  1.00 53.58      A
ATOM   5141  C   GLY A 675    -11.166  35.615  38.151  1.00 53.58      A
ATOM   5142  O   GLY A 675    -10.120  36.262  38.192  1.00 53.58      A
ATOM   5143  N   ALA A 676    -11.189  34.317  37.876  1.00 53.60      A
ATOM   5144  CA  ALA A 676     -9.966  33.593  37.596  1.00 53.60      A
ATOM   5145  CB  ALA A 676     -9.863  32.373  38.511  1.00 39.76      A
ATOM   5146  C   ALA A 676     -9.999  33.161  36.144  1.00 53.60      A
ATOM   5147  O   ALA A 676    -11.070  33.063  35.554  1.00 53.60      A

ATOM   5148  N   ILE A 677     -8.832  32.920  35.558  1.00 48.00      A
ATOM   5149  CA  ILE A 677     -8.773  32.472  34.171  1.00 48.00      A
ATOM   5150  CB  ILE A 677     -7.716  33.245  33.350  1.00 51.13      A
ATOM   5151  CG2 ILE A 677     -7.626  32.656  31.945  1.00 51.13      A
ATOM   5152  CG1 ILE A 677     -8.047  34.741  33.326  1.00 51.13      A
ATOM   5153  CD1 ILE A 677     -9.436  35.080  32.826  1.00 51.13      A
ATOM   5154  C   ILE A 677     -8.399  30.998  34.133  1.00 48.00      A
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FIGURE 25 CON'T

ATOM	5155	O	ILE	A	677	-7.429	30.582	34.771	1.00	48.00	A
ATOM	5156	N	TYR	A	678	-9.171	30.213	33.387	1.00	41.30	A
ATOM	5157	CA	TYR	A	678	-8.911	28.784	33.255	1.00	41.30	A
ATOM	5158	CB	TYR	A	678	-10.199	27.978	33.438	1.00	34.81	A
ATOM	5159	CG	TYR	A	678	-10.693	28.031	34.857	1.00	34.81	A
ATOM	5160	CD1	TYR	A	678	-10.378	27.016	35.770	1.00	34.81	A
ATOM	5161	CE1	TYR	A	678	-10.771	27.101	37.098	1.00	34.81	A
ATOM	5162	CD2	TYR	A	678	-11.419	29.128	35.315	1.00	34.81	A
ATOM	5163	CE2	TYR	A	678	-11.823	29.218	36.642	1.00	34.81	A
ATOM	5164	CZ	TYR	A	678	-11.497	28.205	37.522	1.00	34.81	A
ATOM	5165	OH	TYR	A	678	-11.930	28.288	38.820	1.00	34.81	A
ATOM	5166	C	TYR	A	678	-8.357	28.566	31.874	1.00	41.30	A
ATOM	5167	O	TYR	A	678	-8.950	29.006	30.894	1.00	41.30	A
ATOM	5168	N	LEU	A	679	-7.221	27.884	31.803	1.00	40.92	A
ATOM	5169	CA	LEU	A	679	-6.557	27.637	30.539	1.00	40.92	A
ATOM	5170	CB	LEU	A	679	-5.256	28.450	30.488	1.00	36.79	A
ATOM	5171	CG	LEU	A	679	-4.188	27.964	29.508	1.00	36.79	A
ATOM	5172	CD1	LEU	A	679	-4.568	28.325	28.063	1.00	36.79	A
ATOM	5173	CD2	LEU	A	679	-2.866	28.601	29.883	1.00	36.79	A
ATOM	5174	C	LEU	A	679	-6.239	26.171	30.279	1.00	40.92	A
ATOM	5175	O	LEU	A	679	-5.623	25.505	31.114	1.00	40.92	A
ATOM	5176	N	ILE	A	680	-6.671	25.674	29.124	1.00	44.94	A
ATOM	5177	CA	ILE	A	680	-6.381	24.307	28.712	1.00	44.94	A
ATOM	5178	CB	ILE	A	680	-7.613	23.603	28.079	1.00	45.17	A
ATOM	5179	CG2	ILE	A	680	-7.185	22.297	27.409	1.00	45.17	A
ATOM	5180	CG1	ILE	A	680	-8.664	23.276	29.151	1.00	45.17	A
ATOM	5181	CD1	ILE	A	680	-9.443	24.462	29.677	1.00	45.17	A
ATOM	5182	C	ILE	A	680	-5.275	24.501	27.662	1.00	44.94	A
ATOM	5183	O	ILE	A	680	-5.535	24.935	26.537	1.00	44.94	A
ATOM	5184	N	PRO	A	681	-4.015	24.213	28.038	1.00	59.08	A
ATOM	5185	CD	PRO	A	681	-3.637	23.794	29.398	1.00	62.16	A
ATOM	5186	CA	PRO	A	681	-2.819	24.341	27.195	1.00	59.08	A
ATOM	5187	CB	PRO	A	681	-1.681	23.971	28.149	1.00	62.16	A
ATOM	5188	CG	PRO	A	681	-2.225	24.303	29.490	1.00	62.16	A
ATOM	5189	C	PRO	A	681	-2.795	23.479	25.939	1.00	59.08	A
ATOM	5190	O	PRO	A	681	-2.228	23.868	24.916	1.00	59.08	A
ATOM	5191	N	HIS	A	682	-3.388	22.297	26.029	1.00	56.26	A
ATOM	5192	CA	HIS	A	682	-3.417	21.384	24.895	1.00	56.26	A
ATOM	5193	CB	HIS	A	682	-2.070	20.667	24.776	1.00	89.86	A
ATOM	5194	CG	HIS	A	682	-1.447	20.337	26.098	1.00	89.86	A
ATOM	5195	CD2	HIS	A	682	-0.291	20.755	26.668	1.00	89.86	A
ATOM	5196	ND1	HIS	A	682	-2.044	19.499	27.014	1.00	89.86	A
ATOM	5197	CE1	HIS	A	682	-1.284	19.415	28.092	1.00	89.86	A
ATOM	5198	NE2	HIS	A	682	-0.214	20.168	27.907	1.00	89.86	A
ATOM	5199	C	HIS	A	682	-4.537	20.374	25.055	1.00	56.26	A
ATOM	5200	O	HIS	A	682	-5.056	20.181	26.155	1.00	56.26	A
ATOM	5201	N	LYS	A	683	-4.912	19.734	23.954	1.00	68.26	A
ATOM	5202	CA	LYS	A	683	-5.970	18.735	23.984	1.00	68.26	A
ATOM	5203	CB	LYS	A	683	-6.773	18.774	22.683	1.00	76.15	A
ATOM	5204	CG	LYS	A	683	-5.963	18.410	21.448	1.00	76.15	A
ATOM	5205	CD	LYS	A	683	-6.791	18.519	20.173	1.00	76.15	A
ATOM	5206	CE	LYS	A	683	-7.935	17.519	20.155	1.00	76.15	A
ATOM	5207	NZ	LYS	A	683	-8.770	17.654	18.928	1.00	76.15	A
ATOM	5208	C	LYS	A	683	-5.332	17.365	24.148	1.00	68.26	A
ATOM	5209	O	LYS	A	683	-4.148	17.197	23.868	1.00	68.26	A
ATOM	5210	N	LEU	A	684	-6.110	16.394	24.612	1.00	72.49	A
ATOM	5211	CA	LEU	A	684	-5.605	15.037	24.782	1.00	72.49	A

ATOM	5212	CB	LEU	A	684	-6.517	14.249	25.726	1.00	77.72	A
ATOM	5213	CG	LEU	A	684	-6.837	14.940	27.058	1.00	77.72	A
ATOM	5214	CD1	LEU	A	684	-7.772	14.064	27.872	1.00	77.72	A
ATOM	5215	CD2	LEU	A	684	-5.551	15.220	27.828	1.00	77.72	A
ATOM	5216	C	LEU	A	684	-5.589	14.397	23.392	1.00	72.49	A
ATOM	5217	O	LEU	A	684	-6.638	14.185	22.783	1.00	72.49	A
ATOM	5218	N	LYS	A	685	-4.396	14.094	22.894	1.00	133.17	A
ATOM	5219	CA	LYS	A	685	-4.249	13.521	21.561	1.00	133.17	A
ATOM	5220	CB	LYS	A	685	-2.963	14.055	20.925	1.00	83.35	A
ATOM	5221	CG	LYS	A	685	-2.918	15.575	20.877	1.00	83.35	A
ATOM	5222	CD	LYS	A	685	-1.585	16.102	20.376	1.00	83.35	A
ATOM	5223	CE	LYS	A	685	-1.552	17.624	20.435	1.00	83.35	A
ATOM	5224	NZ	LYS	A	685	-0.230	18.177	20.033	1.00	83.35	A
ATOM	5225	C	LYS	A	685	-4.264	11.997	21.500	1.00	133.17	A
ATOM	5226	O	LYS	A	685	-4.633	11.417	20.478	1.00	133.17	A
ATOM	5227	N	GLN	A	686	-3.874	11.348	22.590	1.00	127.17	A
ATOM	5228	CA	GLN	A	686	-3.840	9.891	22.621	1.00	127.17	A
ATOM	5229	CB	GLN	A	686	-2.389	9.415	22.755	1.00	115.22	A
ATOM	5230	CG	GLN	A	686	-2.193	7.913	22.616	1.00	115.22	A
ATOM	5231	CD	GLN	A	686	-0.734	7.503	22.725	1.00	115.22	A
ATOM	5232	OE1	GLN	A	686	-0.112	7.651	23.778	1.00	115.22	A
ATOM	5233	NE2	GLN	A	686	-0.180	6.991	21.632	1.00	115.22	A
ATOM	5234	C	GLN	A	686	-4.673	9.327	23.765	1.00	127.17	A
ATOM	5235	O	GLN	A	686	-5.658	8.620	23.547	1.00	127.17	A
ATOM	5236	N	ALA	A	687	-4.270	9.660	24.986	1.00	137.90	A
ATOM	5237	CA	ALA	A	687	-4.940	9.182	26.188	1.00	137.90	A
ATOM	5238	CB	ALA	A	687	-4.156	9.627	27.417	1.00	80.16	A
ATOM	5239	C	ALA	A	687	-6.405	9.590	26.332	1.00	137.90	A
ATOM	5240	O	ALA	A	687	-6.863	10.573	25.746	1.00	137.90	A
ATOM	5241	N	LYS	A	688	-7.120	8.804	27.130	1.00	71.04	A
ATOM	5242	CA	LYS	A	688	-8.535	9.002	27.435	1.00	71.04	A
ATOM	5243	CB	LYS	A	688	-9.141	7.650	27.840	1.00	77.29	A
ATOM	5244	CG	LYS	A	688	-10.629	7.631	28.170	1.00	77.29	A
ATOM	5245	CD	LYS	A	688	-11.058	6.193	28.479	1.00	77.29	A
ATOM	5246	CE	LYS	A	688	-12.575	6.019	28.587	1.00	77.29	A
ATOM	5247	NZ	LYS	A	688	-13.181	6.589	29.824	1.00	77.29	A
ATOM	5248	C	LYS	A	688	-8.641	10.002	28.595	1.00	71.04	A
ATOM	5249	O	LYS	A	688	-7.681	10.198	29.342	1.00	71.04	A
ATOM	5250	N	GLY	A	689	-9.797	10.643	28.738	1.00	50.26	A
ATOM	5251	CA	GLY	A	689	-9.965	11.587	29.831	1.00	50.26	A
ATOM	5252	C	GLY	A	689	-10.447	12.966	29.425	1.00	50.26	A
ATOM	5253	O	GLY	A	689	-10.707	13.221	28.251	1.00	50.26	A
ATOM	5254	N	THR	A	690	-10.558	13.852	30.413	1.00	41.72	A
ATOM	5255	CA	THR	A	690	-11.010	15.221	30.205	1.00	41.72	A
ATOM	5256	CB	THR	A	690	-12.225	15.532	31.104	1.00	44.55	A
ATOM	5257	OG1	THR	A	690	-13.314	14.669	30.753	1.00	44.55	A
ATOM	5258	CG2	THR	A	690	-12.665	16.976	30.941	1.00	44.55	A
ATOM	5259	C	THR	A	690	-9.854	16.155	30.558	1.00	41.72	A
ATOM	5260	O	THR	A	690	-9.222	16.003	31.599	1.00	41.72	A
ATOM	5261	N	PRO	A	691	-9.561	17.136	29.692	1.00	42.74	A
ATOM	5262	CD	PRO	A	691	-10.298	17.505	28.471	1.00	43.40	A
ATOM	5263	CA	PRO	A	691	-8.460	18.076	29.946	1.00	42.74	A
ATOM	5264	CB	PRO	A	691	-8.571	19.076	28.794	1.00	43.40	A
ATOM	5265	CG	PRO	A	691	-9.256	18.299	27.710	1.00	43.40	A
ATOM	5266	C	PRO	A	691	-8.573	18.776	31.298	1.00	42.74	A
ATOM	5267	O	PRO	A	691	-9.661	19.157	31.731	1.00	42.74	A
ATOM	5268	N	ILE	A	692	-7.441	18.945	31.965	1.00	47.28	A

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ATOM   5269  CA  ILE A 692      -7.435  19.616  33.245  1.00 47.28      A
ATOM   5270  CB  ILE A 692      -6.587  18.874  34.265  1.00 42.24      A
ATOM   5271  CG2 ILE A 692      -6.732  19.556  35.624  1.00 42.24      A
ATOM   5272  CG1 ILE A 692      -7.028  17.402  34.315  1.00 42.24      A
ATOM   5273  CD1 ILE A 692      -6.274  16.553  35.343  1.00 42.24      A
ATOM   5274  C   ILE A 692      -6.878  21.010  33.051  1.00 47.28      A
ATOM   5275  O   ILE A 692      -5.707  21.180  32.746  1.00 47.28      A

ATOM   5276  N   PRO A 693      -7.725  22.032  33.224  1.00 45.32      A
ATOM   5277  CD  PRO A 693      -9.147  21.972  33.594  1.00 36.54      A
ATOM   5278  CA  PRO A 693      -7.287  23.416  33.055  1.00 45.32      A
ATOM   5279  CB  PRO A 693      -8.592  24.223  33.135  1.00 36.54      A
ATOM   5280  CG  PRO A 693      -9.690  23.205  32.926  1.00 36.54      A
ATOM   5281  C   PRO A 693      -6.334  23.861  34.147  1.00 45.32      A
ATOM   5282  O   PRO A 693      -6.356  23.340  35.260  1.00 45.32      A
ATOM   5283  N   ILE A 694      -5.504  24.840  33.819  1.00 38.05      A
ATOM   5284  CA  ILE A 694      -4.620  25.424  34.802  1.00 38.05      A
ATOM   5285  CB  ILE A 694      -3.313  25.934  34.178  1.00 57.89      A
ATOM   5286  CG2 ILE A 694      -2.505  26.688  35.220  1.00 57.89      A
ATOM   5287  CG1 ILE A 694      -2.511  24.769  33.616  1.00 57.89      A
ATOM   5288  CD1 ILE A 694      -1.279  25.216  32.844  1.00 57.89      A
ATOM   5289  C   ILE A 694      -5.423  26.641  35.232  1.00 38.05      A
ATOM   5290  O   ILE A 694      -5.916  27.378  34.378  1.00 38.05      A
ATOM   5291  N   LYS A 695      -5.551  26.864  36.535  1.00 40.66      A
ATOM   5292  CA  LYS A 695      -6.286  28.010  37.034  1.00 40.66      A
ATOM   5293  CB  LYS A 695      -7.098  27.591  38.256  1.00 39.88      A
ATOM   5294  CG  LYS A 695      -7.929  28.690  38.877  1.00 39.88      A
ATOM   5295  CD  LYS A 695      -8.674  28.164  40.097  1.00 39.88      A
ATOM   5296  CE  LYS A 695      -9.491  29.258  40.772  1.00 39.88      A
ATOM   5297  NZ  LYS A 695     -10.134  28.753  42.038  1.00 39.88      A
ATOM   5298  C   LYS A 695      -5.317  29.155  37.392  1.00 40.66      A
ATOM   5299  O   LYS A 695      -4.383  28.978  38.188  1.00 40.66      A
ATOM   5300  N   LEU A 696      -5.537  30.325  36.793  1.00 47.41      A
ATOM   5301  CA  LEU A 696      -4.693  31.492  37.032  1.00 47.41      A
ATOM   5302  CB  LEU A 696      -4.206  32.072  35.705  1.00 40.52      A
ATOM   5303  CG  LEU A 696      -3.545  31.121  34.723  1.00 40.52      A
ATOM   5304  CD1 LEU A 696      -3.303  31.831  33.394  1.00 40.52      A
ATOM   5305  CD2 LEU A 696      -2.245  30.620  35.321  1.00 40.52      A
ATOM   5306  C   LEU A 696      -5.500  32.549  37.766  1.00 47.41      A
ATOM   5307  O   LEU A 696      -6.610  32.872  37.344  1.00 47.41      A
ATOM   5308  N   ALA A 697      -4.955  33.091  38.858  1.00 44.29      A
ATOM   5309  CA  ALA A 697      -5.683  34.109  39.616  1.00 44.29      A
ATOM   5310  CB  ALA A 697      -6.798  33.446  40.404  1.00 65.48      A
ATOM   5311  C   ALA A 697      -4.845  34.989  40.557  1.00 44.29      A
ATOM   5312  O   ALA A 697      -3.669  34.710  40.827  1.00 44.29      A
ATOM   5313  N   LYS A 698      -5.481  36.053  41.051  1.00 43.91      A
ATOM   5314  CA  LYS A 698      -4.869  36.994  41.982  1.00 43.91      A
ATOM   5315  CB  LYS A 698      -4.782  36.372  43.379  1.00 72.05      A
ATOM   5316  CG  LYS A 698      -6.125  35.997  43.975  1.00 72.05      A
ATOM   5317  CD  LYS A 698      -5.951  35.321  45.324  1.00 72.05      A
ATOM   5318  CE  LYS A 698      -7.290  34.913  45.917  1.00 72.05      A
ATOM   5319  NZ  LYS A 698      -7.120  34.130  47.182  1.00 72.05      A
ATOM   5320  C   LYS A 698      -3.489  37.459  41.553  1.00 43.91      A
ATOM   5321  O   LYS A 698      -2.544  37.414  42.331  1.00 43.91      A
ATOM   5322  N   LYS A 699      -3.373  37.899  40.309  1.00 59.17      A
ATOM   5323  CA  LYS A 699      -2.109  38.386  39.801  1.00 59.17      A
ATOM   5324  CB  LYS A 699      -2.236  38.668  38.308  1.00 58.69      A
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FIGURE 25 CON'T

ATOM	5325	CG	LYS	A	699	-0.983	39.210	37.659	1.00	58.69	A
ATOM	5326	CD	LYS	A	699	-1.126	39.200	36.145	1.00	58.69	A
ATOM	5327	CE	LYS	A	699	0.087	39.802	35.475	1.00	58.69	A
ATOM	5328	NZ	LYS	A	699	0.275	41.205	35.928	1.00	58.69	A
ATOM	5329	C	LYS	A	699	-1.788	39.666	40.559	1.00	59.17	A
ATOM	5330	O	LYS	A	699	-2.690	40.337	41.058	1.00	59.17	A
ATOM	5331	N	ARG	A	700	-0.509	39.997	40.675	1.00	53.00	A
ATOM	5332	CA	ARG	A	700	-0.119	41.212	41.375	1.00	53.00	A
ATOM	5333	CB	ARG	A	700	-0.174	40.998	42.884	1.00	71.74	A
ATOM	5334	CG	ARG	A	700	0.951	40.143	43.410	1.00	71.74	A
ATOM	5335	CD	ARG	A	700	0.809	39.858	44.896	1.00	71.74	A
ATOM	5336	NE	ARG	A	700	-0.252	38.902	45.223	1.00	71.74	A
ATOM	5337	CZ	ARG	A	700	-0.420	37.724	44.629	1.00	71.74	A
ATOM	5338	NH1	ARG	A	700	0.394	37.343	43.655	1.00	71.74	A
ATOM	5339	NH2	ARG	A	700	-1.380	36.904	45.032	1.00	71.74	A
ATOM	5340	C	ARG	A	700	1.286	41.619	40.958	1.00	53.00	A
ATOM	5341	O	ARG	A	700	2.062	40.798	40.463	1.00	53.00	A
ATOM	5342	N	ILE	A	701	1.605	42.896	41.142	1.00	59.98	A
ATOM	5343	CA	ILE	A	701	2.925	43.417	40.797	1.00	59.98	A
ATOM	5344	CB	ILE	A	701	2.824	44.566	39.780	1.00	73.76	A
ATOM	5345	CG2	ILE	A	701	1.938	45.668	40.332	1.00	73.76	A
ATOM	5346	CG1	ILE	A	701	4.213	45.131	39.485	1.00	73.76	A
ATOM	5347	CD1	ILE	A	701	5.133	44.162	38.812	1.00	73.76	A
ATOM	5348	C	ILE	A	701	3.563	43.948	42.071	1.00	59.98	A
ATOM	5349	O	ILE	A	701	2.904	44.593	42.881	1.00	59.98	A
ATOM	5350	N	ILE	A	702	4.844	43.670	42.258	1.00	61.88	A
ATOM	5351	CA	ILE	A	702	5.521	44.139	43.452	1.00	61.88	A
ATOM	5352	CB	ILE	A	702	5.989	42.956	44.330	1.00	70.36	A
ATOM	5353	CG2	ILE	A	702	6.488	43.471	45.676	1.00	70.36	A
ATOM	5354	CG1	ILE	A	702	4.822	41.989	44.558	1.00	70.36	A
ATOM	5355	CD1	ILE	A	702	5.168	40.803	45.437	1.00	70.36	A
ATOM	5356	C	ILE	A	702	6.714	45.001	43.073	1.00	61.88	A
ATOM	5357	O	ILE	A	702	7.685	44.511	42.501	1.00	61.88	A
ATOM	5358	N	LYS	A	703	6.617	46.291	43.387	1.00	76.24	A
ATOM	5359	CA	LYS	A	703	7.673	47.257	43.094	1.00	76.24	A
ATOM	5360	CB	LYS	A	703	7.181	48.332	42.122	1.00	89.04	A
ATOM	5361	CG	LYS	A	703	6.615	47.828	40.814	1.00	89.04	A
ATOM	5362	CD	LYS	A	703	6.088	48.998	39.991	1.00	89.04	A
ATOM	5363	CE	LYS	A	703	5.294	48.536	38.777	1.00	89.04	A
ATOM	5364	NZ	LYS	A	703	4.798	49.691	37.972	1.00	89.04	A
ATOM	5365	C	LYS	A	703	8.089	47.940	44.388	1.00	76.24	A
ATOM	5366	O	LYS	A	703	7.247	48.284	45.217	1.00	76.24	A
ATOM	5367	N	ASN	A	704	9.391	48.137	44.552	1.00	76.83	A
ATOM	5368	CA	ASN	A	704	9.920	48.797	45.735	1.00	76.83	A
ATOM	5369	CB	ASN	A	704	9.793	50.312	45.573	1.00	83.90	A
ATOM	5370	CG	ASN	A	704	10.302	50.794	44.229	1.00	83.90	A
ATOM	5371	OD1	ASN	A	704	11.483	50.642	43.905	1.00	83.90	A
ATOM	5372	ND2	ASN	A	704	9.409	51.369	43.433	1.00	83.90	A
ATOM	5373	C	ASN	A	704	9.218	48.351	47.015	1.00	76.83	A
ATOM	5374	O	ASN	A	704	8.875	49.173	47.868	1.00	76.83	A
ATOM	5375	N	GLY	A	705	8.987	47.046	47.132	1.00	60.58	A
ATOM	5376	CA	GLY	A	705	8.357	46.504	48.324	1.00	60.58	A
ATOM	5377	C	GLY	A	705	6.867	46.724	48.461	1.00	60.58	A
ATOM	5378	O	GLY	A	705	6.284	46.380	49.492	1.00	60.58	A
ATOM	5379	N	LYS	A	706	6.241	47.285	47.434	1.00	69.84	A
ATOM	5380	CA	LYS	A	706	4.805	47.533	47.479	1.00	69.84	A
ATOM	5381	CB	LYS	A	706	4.514	49.008	47.190	1.00	118.05	A

FIGURE 25 CON'T

ATOM	5382	CG	LYS	A	706	4.906	49.937	48.328	1.00118.05	A
ATOM	5383	CD	LYS	A	706	4.159	49.575	49.605	1.00118.05	A
ATOM	5384	CE	LYS	A	706	4.587	50.451	50.771	1.00118.05	A
ATOM	5385	NZ	LYS	A	706	3.854	50.103	52.022	1.00118.05	A
ATOM	5386	C	LYS	A	706	4.011	46.644	46.525	1.00 69.84	A
ATOM	5387	O	LYS	A	706	4.396	46.444	45.368	1.00 69.84	A
ATOM	5388	N	VAL	A	707	2.891	46.126	47.028	1.00 58.45	A
ATOM	5389	CA	VAL	A	707	2.021	45.242	46.262	1.00 58.45	A
ATOM	5390	CB	VAL	A	707	1.510	44.085	47.139	1.00 55.42	A
ATOM	5391	CG1	VAL	A	707	0.611	43.165	46.316	1.00 55.42	A
ATOM	5392	CG2	VAL	A	707	2.686	43.322	47.713	1.00 55.42	A
ATOM	5393	C	VAL	A	707	0.806	45.942	45.654	1.00 58.45	A
ATOM	5394	O	VAL	A	707	0.056	46.638	46.341	1.00 58.45	A
ATOM	5395	N	GLU	A	708	0.613	45.728	44.358	1.00 65.11	A
ATOM	5396	CA	GLU	A	708	-0.505	46.314	43.638	1.00 65.11	A
ATOM	5397	CB	GLU	A	708	0.009	47.375	42.662	1.00156.55	A
ATOM	5398	CG	GLU	A	708	0.849	48.454	43.329	1.00156.55	A
ATOM	5399	CD	GLU	A	708	1.445	49.432	42.337	1.00156.55	A
ATOM	5400	OE1	GLU	A	708	2.219	48.992	41.461	1.00156.55	A
ATOM	5401	OE2	GLU	A	708	1.142	50.639	42.437	1.00156.55	A
ATOM	5402	C	GLU	A	708	-1.254	45.221	42.879	1.00 65.11	A
ATOM	5403	O	GLU	A	708	-0.801	44.759	41.831	1.00 65.11	A
ATOM	5404	N	LYS	A	709	-2.396	44.805	43.419	1.00 65.35	A
ATOM	5405	CA	LYS	A	709	-3.209	43.768	42.789	1.00 65.35	A
ATOM	5406	CB	LYS	A	709	-4.548	43.622	43.511	1.00 70.74	A
ATOM	5407	CG	LYS	A	709	-4.436	43.305	44.994	1.00 70.74	A
ATOM	5408	CD	LYS	A	709	-5.814	43.089	45.594	1.00 70.74	A
ATOM	5409	CE	LYS	A	709	-5.747	42.919	47.099	1.00 70.74	A
ATOM	5410	NZ	LYS	A	709	-7.099	42.643	47.674	1.00 70.74	A
ATOM	5411	C	LYS	A	709	-3.459	44.150	41.342	1.00 65.35	A
ATOM	5412	O	LYS	A	709	-3.913	45.256	41.063	1.00 65.35	A
ATOM	5413	N	GLN	A	710	-3.158	43.240	40.422	1.00 72.53	A
ATOM	5414	CA	GLN	A	710	-3.349	43.518	39.006	1.00 72.53	A
ATOM	5415	CB	GLN	A	710	-2.044	43.291	38.239	1.00112.53	A
ATOM	5416	CG	GLN	A	710	-1.769	44.344	37.178	1.00112.53	A
ATOM	5417	CD	GLN	A	710	-1.363	45.681	37.779	1.00112.53	A
ATOM	5418	OE1	GLN	A	710	-0.239	45.845	38.252	1.00112.53	A
ATOM	5419	NE2	GLN	A	710	-2.281	46.641	37.770	1.00112.53	A
ATOM	5420	C	GLN	A	710	-4.445	42.635	38.421	1.00 72.53	A
ATOM	5421	O	GLN	A	710	-5.155	41.940	39.153	1.00 72.53	A
ATOM	5422	N	SER	A	711	-4.583	42.676	37.100	1.00 67.00	A
ATOM	5423	CA	SER	A	711	-5.580	41.879	36.407	1.00 67.00	A
ATOM	5424	CB	SER	A	711	-6.606	42.787	35.725	1.00106.90	A
ATOM	5425	OG	SER	A	711	-7.311	43.564	36.677	1.00106.90	A
ATOM	5426	C	SER	A	711	-4.870	41.025	35.369	1.00 67.00	A
ATOM	5427	O	SER	A	711	-3.918	41.481	34.737	1.00 67.00	A
ATOM	5428	N	ILE	A	712	-5.327	39.787	35.203	1.00 59.42	A
ATOM	5429	CA	ILE	A	712	-4.720	38.876	34.244	1.00 59.42	A
ATOM	5430	CB	ILE	A	712	-5.131	37.410	34.543	1.00 44.31	A
ATOM	5431	CG2	ILE	A	712	-4.562	36.465	33.476	1.00 44.31	A
ATOM	5432	CG1	ILE	A	712	-4.627	37.019	35.939	1.00 44.31	A
ATOM	5433	CD1	ILE	A	712	-5.076	35.659	36.406	1.00 44.31	A
ATOM	5434	C	ILE	A	712	-5.164	39.291	32.846	1.00 59.42	A
ATOM	5435	O	ILE	A	712	-6.334	39.621	32.636	1.00 59.42	A
ATOM	5436	N	THR	A	713	-4.220	39.278	31.905	1.00 58.31	A
ATOM	5437	CA	THR	A	713	-4.469	39.685	30.527	1.00 58.31	A

FIGURE 25 CON'T

ATOM	5438	CB	THR	A	713	-3.509	40.806	30.107	1.00	60.66	A
ATOM	5439	OG1	THR	A	713	-2.184	40.266	29.989	1.00	60.66	A
ATOM	5440	CG2	THR	A	713	-3.501	41.922	31.140	1.00	60.66	A
ATOM	5441	C	THR	A	713	-4.275	38.545	29.541	1.00	58.31	A
ATOM	5442	O	THR	A	713	-3.750	37.484	29.883	1.00	58.31	A
ATOM	5443	N	ARG	A	714	-4.690	38.774	28.304	1.00	56.92	A
ATOM	5444	CA	ARG	A	714	-4.542	37.759	27.281	1.00	56.92	A
ATOM	5445	CB	ARG	A	714	-5.152	38.236	25.963	1.00	101.08	A
ATOM	5446	CG	ARG	A	714	-6.647	38.453	26.038	1.00	101.08	A
ATOM	5447	CD	ARG	A	714	-7.249	38.679	24.667	1.00	101.08	A
ATOM	5448	NE	ARG	A	714	-8.703	38.774	24.735	1.00	101.08	A
ATOM	5449	CZ	ARG	A	714	-9.498	38.851	23.674	1.00	101.08	A
ATOM	5450	NH1	ARG	A	714	-8.982	38.844	22.451	1.00	101.08	A
ATOM	5451	NH2	ARG	A	714	-10.812	38.929	23.837	1.00	101.08	A
ATOM	5452	C	ARG	A	714	-3.060	37.457	27.099	1.00	56.92	A
ATOM	5453	O	ARG	A	714	-2.677	36.314	26.847	1.00	56.92	A
ATOM	5454	N	GLN	A	715	-2.231	38.489	27.227	1.00	57.29	A
ATOM	5455	CA	GLN	A	715	-0.787	38.331	27.092	1.00	57.29	A
ATOM	5456	CB	GLN	A	715	-0.086	39.689	27.192	1.00	91.22	A
ATOM	5457	CG	GLN	A	715	0.676	40.091	25.933	1.00	91.22	A
ATOM	5458	CD	GLN	A	715	1.793	39.121	25.584	1.00	91.22	A
ATOM	5459	OE1	GLN	A	715	2.695	38.886	26.385	1.00	91.22	A
ATOM	5460	NE2	GLN	A	715	1.739	38.559	24.382	1.00	91.22	A
ATOM	5461	C	GLN	A	715	-0.262	37.397	28.184	1.00	57.29	A
ATOM	5462	O	GLN	A	715	0.594	36.554	27.925	1.00	57.29	A
ATOM	5463	N	ASP	A	716	-0.779	37.558	29.397	1.00	55.13	A
ATOM	5464	CA	ASP	A	716	-0.382	36.714	30.522	1.00	55.13	A
ATOM	5465	CB	ASP	A	716	-1.094	37.150	31.805	1.00	51.94	A
ATOM	5466	CG	ASP	A	716	-0.634	38.507	32.297	1.00	51.94	A
ATOM	5467	OD1	ASP	A	716	0.550	38.848	32.095	1.00	51.94	A
ATOM	5468	OD2	ASP	A	716	-1.455	39.232	32.903	1.00	51.94	A
ATOM	5469	C	ASP	A	716	-0.717	35.254	30.234	1.00	55.13	A
ATOM	5470	O	ASP	A	716	0.080	34.354	30.518	1.00	55.13	A
ATOM	5471	N	VAL	A	717	-1.899	35.028	29.664	1.00	45.86	A
ATOM	5472	CA	VAL	A	717	-2.344	33.682	29.332	1.00	45.86	A
ATOM	5473	CB	VAL	A	717	-3.820	33.686	28.836	1.00	41.48	A
ATOM	5474	CG1	VAL	A	717	-4.220	32.289	28.340	1.00	41.48	A
ATOM	5475	CG2	VAL	A	717	-4.749	34.154	29.965	1.00	41.48	A
ATOM	5476	C	VAL	A	717	-1.435	33.119	28.249	1.00	45.86	A
ATOM	5477	O	VAL	A	717	-1.135	31.918	28.228	1.00	45.86	A
ATOM	5478	N	LEU	A	718	-0.992	33.989	27.350	1.00	48.09	A
ATOM	5479	CA	LEU	A	718	-0.096	33.575	26.267	1.00	48.09	A
ATOM	5480	CB	LEU	A	718	0.150	34.740	25.300	1.00	64.92	A
ATOM	5481	CG	LEU	A	718	0.401	34.446	23.815	1.00	64.92	A
ATOM	5482	CD1	LEU	A	718	0.989	35.702	23.173	1.00	64.92	A
ATOM	5483	CD2	LEU	A	718	1.349	33.281	23.625	1.00	64.92	A
ATOM	5484	C	LEU	A	718	1.249	33.136	26.870	1.00	48.09	A
ATOM	5485	O	LEU	A	718	1.821	32.127	26.459	1.00	48.09	A
ATOM	5486	N	ASP	A	719	1.754	33.907	27.830	1.00	48.83	A
ATOM	5487	CA	ASP	A	719	3.021	33.569	28.475	1.00	48.83	A
ATOM	5488	CB	ASP	A	719	3.395	34.617	29.532	1.00	48.69	A
ATOM	5489	CG	ASP	A	719	3.735	35.981	28.926	1.00	48.69	A
ATOM	5490	OD1	ASP	A	719	4.239	36.028	27.779	1.00	48.69	A
ATOM	5491	OD2	ASP	A	719	3.518	37.008	29.608	1.00	48.69	A
ATOM	5492	C	ASP	A	719	2.907	32.187	29.134	1.00	48.83	A
ATOM	5493	O	ASP	A	719	3.697	31.281	28.842	1.00	48.83	A
ATOM	5494	N	ILE	A	720	1.916	32.024	30.012	1.00	43.40	A

FIGURE 25 CON'T

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ATOM   5495  CA  ILE A 720       1.713  30.746  30.686  1.00 43.40      A
ATOM   5496  CB  ILE A 720       0.407  30.734  31.507  1.00 41.33      A
ATOM   5497  CG2 ILE A 720       0.146  29.326  32.050  1.00 41.33      A
ATOM   5498  CG1 ILE A 720       0.506  31.741  32.648  1.00 41.33      A
ATOM   5499  CD1 ILE A 720       1.710  31.509  33.584  1.00 41.33      A
ATOM   5500  C   ILE A 720       1.639  29.646  29.646  1.00 43.40      A
ATOM   5501  O   ILE A 720       2.271  28.596  29.781  1.00 43.40      A
ATOM   5502  N   PHE A 721       0.872  29.904  28.594  1.00 42.36      A
ATOM   5503  CA  PHE A 721       0.717  28.938  27.518  1.00 42.36      A
ATOM   5504  CB  PHE A 721      -0.127  29.518  26.382  1.00 49.57      A
ATOM   5505  CG  PHE A 721      -0.237  28.604  25.199  1.00 49.57      A
ATOM   5506  CD1 PHE A 721      -1.096  27.515  25.226  1.00 49.57      A
ATOM   5507  CD2 PHE A 721       0.539  28.819  24.064  1.00 49.57      A
ATOM   5508  CE1 PHE A 721      -1.186  26.649  24.134  1.00 49.57      A
ATOM   5509  CE2 PHE A 721       0.458  27.963  22.973  1.00 49.57      A
ATOM   5510  CZ  PHE A 721      -0.407  26.874  23.004  1.00 49.57      A
ATOM   5511  C   PHE A 721       2.061  28.509  26.949  1.00 42.36      A
ATOM   5512  O   PHE A 721       2.331  27.312  26.804  1.00 42.36      A
ATOM   5513  N   ILE A 722       2.899  29.482  26.608  1.00 51.86      A
ATOM   5514  CA  ILE A 722       4.203  29.162  26.041  1.00 51.86      A
ATOM   5515  CB  ILE A 722       4.981  30.446  25.634  1.00 49.95      A
ATOM   5516  CG2 ILE A 722       6.258  30.070  24.893  1.00 49.95      A
ATOM   5517  CG1 ILE A 722       4.120  31.306  24.703  1.00 49.95      A
ATOM   5518  CD1 ILE A 722       3.723  30.615  23.418  1.00 49.95      A
ATOM   5519  C   ILE A 722       5.020  28.355  27.051  1.00 51.86      A
ATOM   5520  O   ILE A 722       5.552  27.296  26.722  1.00 51.86      A
ATOM   5521  N   LEU A 723       5.093  28.848  28.282  1.00 50.06      A
ATOM   5522  CA  LEU A 723       5.837  28.174  29.341  1.00 50.06      A
ATOM   5523  CB  LEU A 723       5.687  28.939  30.653  1.00 43.52      A
ATOM   5524  CG  LEU A 723       6.300  30.340  30.634  1.00 43.52      A
ATOM   5525  CD1 LEU A 723       6.051  31.040  31.970  1.00 43.52      A
ATOM   5526  CD2 LEU A 723       7.802  30.226  30.347  1.00 43.52      A
ATOM   5527  C   LEU A 723       5.383  26.736  29.535  1.00 50.06      A
ATOM   5528  O   LEU A 723       6.153  25.883  29.982  1.00 50.06      A
ATOM   5529  N   THR A 724       4.126  26.466  29.205  1.00 48.74      A
ATOM   5530  CA  THR A 724       3.598  25.121  29.340  1.00 48.74      A
ATOM   5531  CB  THR A 724       2.056  25.140  29.419  1.00 65.45      A

ATOM   5532  OG1 THR A 724       1.655  25.818  30.616  1.00 65.45      A
ATOM   5533  CG2 THR A 724       1.502  23.730  29.447  1.00 65.45      A
ATOM   5534  C   THR A 724       4.036  24.226  28.188  1.00 48.74      A
ATOM   5535  O   THR A 724       4.061  23.006  28.327  1.00 48.74      A
ATOM   5536  N   ARG A 725       4.387  24.820  27.051  1.00 47.84      A
ATOM   5537  CA  ARG A 725       4.815  24.021  25.903  1.00 47.84      A
ATOM   5538  CB  ARG A 725       4.466  24.742  24.595  1.00 76.71      A
ATOM   5539  CG  ARG A 725       2.969  24.777  24.302  1.00 76.71      A
ATOM   5540  CD  ARG A 725       2.377  23.391  24.508  1.00 76.71      A
ATOM   5541  NE  ARG A 725       0.969  23.300  24.145  1.00 76.71      A
ATOM   5542  CZ  ARG A 725       0.525  23.274  22.895  1.00 76.71      A
ATOM   5543  NH1 ARG A 725       1.382  23.335  21.883  1.00 76.71      A
ATOM   5544  NH2 ARG A 725      -0.775  23.171  22.659  1.00 76.71      A
ATOM   5545  C   ARG A 725       6.297  23.635  25.910  1.00 47.84      A
ATOM   5546  O   ARG A 725       6.771  22.967  24.999  1.00 47.84      A
ATOM   5547  N   LEU A 726       7.029  24.048  26.938  1.00 53.00      A
ATOM   5548  CA  LEU A 726       8.444  23.702  27.031  1.00 53.00      A
ATOM   5549  CB  LEU A 726       9.206  24.873  27.672  1.00 47.46      A
ATOM   5550  CG  LEU A 726       9.077  26.189  26.878  1.00 47.46      A
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FIGURE 25 CON'T

ATOM	5551	CD1	LEU	A	726	9.639	27.362	27.667	1.00	47.46	A
ATOM	5552	CD2	LEU	A	726	9.813	26.053	25.542	1.00	47.46	A
ATOM	5553	C	LEU	A	726	8.584	22.397	27.844	1.00	53.00	A
ATOM	5554	O	LEU	A	726	8.942	22.414	29.019	1.00	53.00	A
ATOM	5555	N	ASN	A	727	8.288	21.271	27.189	1.00	53.74	A
ATOM	5556	CA	ASN	A	727	8.323	19.937	27.802	1.00	53.74	A
ATOM	5557	CB	ASN	A	727	7.077	19.153	27.384	1.00	71.67	A
ATOM	5558	CG	ASN	A	727	7.085	18.795	25.907	1.00	71.67	A
ATOM	5559	OD1	ASN	A	727	7.386	19.628	25.057	1.00	71.67	A
ATOM	5560	ND2	ASN	A	727	6.748	17.551	25.597	1.00	71.67	A
ATOM	5561	C	ASN	A	727	9.567	19.083	27.493	1.00	53.74	A
ATOM	5562	O	ASN	A	727	9.668	17.931	27.935	1.00	53.74	A
ATOM	5563	N	TYR	A	728	10.482	19.623	26.696	1.00	54.75	A
ATOM	5564	CA	TYR	A	728	11.730	18.928	26.378	1.00	54.75	A
ATOM	5565	CB	TYR	A	728	12.662	19.060	27.586	1.00	56.67	A
ATOM	5566	CG	TYR	A	728	12.969	20.502	27.924	1.00	56.67	A
ATOM	5567	CD1	TYR	A	728	14.024	21.172	27.302	1.00	56.67	A
ATOM	5568	CE1	TYR	A	728	14.284	22.502	27.570	1.00	56.67	A
ATOM	5569	CD2	TYR	A	728	12.178	21.211	28.827	1.00	56.67	A
ATOM	5570	CE2	TYR	A	728	12.427	22.550	29.100	1.00	56.67	A
ATOM	5571	CZ	TYR	A	728	13.484	23.186	28.469	1.00	56.67	A
ATOM	5572	OH	TYR	A	728	13.759	24.507	28.744	1.00	56.67	A
ATOM	5573	C	TYR	A	728	11.666	17.451	25.937	1.00	54.75	A
ATOM	5574	O	TYR	A	728	12.359	16.601	26.503	1.00	54.75	A
ATOM	5575	N	GLY	A	729	10.843	17.152	24.932	1.00	54.03	A
ATOM	5576	CA	GLY	A	729	10.749	15.788	24.426	1.00	54.03	A
ATOM	5577	C	GLY	A	729	9.915	14.783	25.208	1.00	54.03	A
ATOM	5578	O	GLY	A	729	9.689	13.665	24.738	1.00	54.03	A
ATOM	5579	N	SER	A	730	9.452	15.173	26.389	1.00	62.98	A
ATOM	5580	CA	SER	A	730	8.651	14.288	27.223	1.00	62.98	A
ATOM	5581	CB	SER	A	730	8.218	15.018	28.496	1.00	89.59	A
ATOM	5582	OG	SER	A	730	7.491	14.151	29.347	1.00	89.59	A
ATOM	5583	C	SER	A	730	7.415	13.766	26.481	1.00	62.98	A
ATOM	5584	O	SER	A	730	6.368	14.420	26.449	1.00	62.98	A
ATOM	5585	N	ILE	A	731	7.551	12.586	25.883	1.00141.32		A
ATOM	5586	CA	ILE	A	731	6.449	11.974	25.153	1.00141.32		A
ATOM	5587	CB	ILE	A	731	6.811	10.547	24.694	1.00122.31		A
ATOM	5588	CG2	ILE	A	731	5.704	9.993	23.805	1.00122.31		A
ATOM	5589	CG1	ILE	A	731	8.140	10.569	23.933	1.00122.31		A
ATOM	5590	CD1	ILE	A	731	8.674	9.194	23.581	1.00122.31		A
ATOM	5591	C	ILE	A	731	5.246	11.918	26.088	1.00141.32		A
ATOM	5592	O	ILE	A	731	5.403	11.765	27.301	1.00141.32		A
ATOM	5593	N	SER	A	732	4.049	12.047	25.523	1.00191.41		A
ATOM	5594	CA	SER	A	732	2.821	12.035	26.310	1.00191.41		A
ATOM	5595	CB	SER	A	732	2.764	10.790	27.203	1.00119.32		A
ATOM	5596	OG	SER	A	732	2.817	9.604	26.430	1.00119.32		A
ATOM	5597	C	SER	A	732	2.786	13.296	27.171	1.00191.41		A
ATOM	5598	O	SER	A	732	2.926	13.233	28.393	1.00191.41		A
ATOM	5599	N	ALA	A	733	2.606	14.440	26.517	1.00174.30		A
ATOM	5600	CA	ALA	A	733	2.562	15.731	27.197	1.00174.30		A
ATOM	5601	CB	ALA	A	733	2.309	16.843	26.182	1.00	95.05	A
ATOM	5602	C	ALA	A	733	1.505	15.777	28.297	1.00174.30		A
ATOM	5603	O	ALA	A	733	0.314	15.939	28.026	1.00174.30		A
ATOM	5604	N	ASP	A	734	1.953	15.636	29.540	1.00130.52		A
ATOM	5605	CA	ASP	A	734	1.056	15.669	30.687	1.00130.52		A
ATOM	5606	CB	ASP	A	734	1.081	14.325	31.415	1.00142.65		A
ATOM	5607	CG	ASP	A	734	0.587	13.188	30.546	1.00142.65		A

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ATOM	5608	OD1	ASP	A	734	-0.587	13.230	30.123	1.00142.65	A
ATOM	5609	OD2	ASP	A	734	1.374	12.254	30.284	1.00142.65	A
ATOM	5610	C	ASP	A	734	1.469	16.783	31.640	1.00130.52	A
ATOM	5611	O	ASP	A	734	0.830	17.001	32.671	1.00130.52	A
ATOM	5612	N	MSE	A	735	2.544	17.484	31.286	1.00 83.68	A
ATOM	5613	CA	MSE	A	735	3.045	18.586	32.100	1.00 83.68	A
ATOM	5614	CB	MSE	A	735	4.291	19.200	31.441	1.00 77.09	A
ATOM	5615	CG	MSE	A	735	5.145	20.077	32.359	1.00 77.09	A
ATOM	5616	SE	MSE	A	735	6.711	20.840	31.466	1.00 77.09	A
ATOM	5617	CE	MSE	A	735	7.603	19.190	30.986	1.00 77.09	A
ATOM	5618	C	MSE	A	735	1.924	19.620	32.193	1.00 83.68	A
ATOM	5619	O	MSE	A	735	1.658	20.350	31.239	1.00 83.68	A
ATOM	5620	N	ARG	A	736	1.255	19.665	33.339	1.00 86.57	A
ATOM	5621	CA	ARG	A	736	0.157	20.605	33.533	1.00 86.57	A
ATOM	5622	CB	ARG	A	736	-0.890	20.006	34.483	1.00 66.03	A
ATOM	5623	CG	ARG	A	736	-2.275	20.667	34.409	1.00 66.03	A
ATOM	5624	CD	ARG	A	736	-3.147	20.224	35.570	1.00 66.03	A
ATOM	5625	NE	ARG	A	736	-2.995	18.798	35.836	1.00 66.03	A
ATOM	5626	CZ	ARG	A	736	-3.511	18.172	36.889	1.00 66.03	A
ATOM	5627	NH1	ARG	A	736	-4.220	18.845	37.785	1.00 66.03	A
ATOM	5628	NH2	ARG	A	736	-3.307	16.870	37.056	1.00 66.03	A
ATOM	5629	C	ARG	A	736	0.655	21.927	34.109	1.00 86.57	A
ATOM	5630	O	ARG	A	736	-0.139	22.821	34.395	1.00 86.57	A
ATOM	5631	N	LEU	A	737	1.968	22.057	34.278	1.00 43.91	A
ATOM	5632	CA	LEU	A	737	2.520	23.284	34.850	1.00 43.91	A
ATOM	5633	CB	LEU	A	737	3.191	22.987	36.191	1.00 59.16	A
ATOM	5634	CG	LEU	A	737	2.353	22.572	37.395	1.00 59.16	A
ATOM	5635	CD1	LEU	A	737	3.286	22.259	38.543	1.00 59.16	A
ATOM	5636	CD2	LEU	A	737	1.395	23.680	37.777	1.00 59.16	A
ATOM	5637	C	LEU	A	737	3.531	23.980	33.977	1.00 43.91	A
ATOM	5638	O	LEU	A	737	4.164	23.362	33.123	1.00 43.91	A
ATOM	5639	N	PRO	A	738	3.680	25.299	34.163	1.00 43.31	A
ATOM	5640	CD	PRO	A	738	2.886	26.184	35.032	1.00 37.96	A
ATOM	5641	CA	PRO	A	738	4.653	26.073	33.386	1.00 43.31	A
ATOM	5642	CB	PRO	A	738	4.562	27.454	34.021	1.00 37.96	A
ATOM	5643	CG	PRO	A	738	3.115	27.525	34.416	1.00 37.96	A
ATOM	5644	C	PRO	A	738	6.011	25.410	33.644	1.00 43.31	A
ATOM	5645	O	PRO	A	738	6.336	25.082	34.786	1.00 43.31	A
ATOM	5646	N	ALA	A	739	6.787	25.206	32.584	1.00 39.08	A
ATOM	5647	CA	ALA	A	739	8.091	24.557	32.685	1.00 39.08	A
ATOM	5648	CB	ALA	A	739	8.862	24.765	31.385	1.00 30.43	A
ATOM	5649	C	ALA	A	739	8.949	25.001	33.878	1.00 39.08	A
ATOM	5650	O	ALA	A	739	9.495	24.175	34.587	1.00 39.08	A
ATOM	5651	N	PRO	A	740	9.082	26.315	34.111	1.00 39.59	A
ATOM	5652	CD	PRO	A	740	8.523	27.468	33.389	1.00 52.42	A
ATOM	5653	CA	PRO	A	740	9.908	26.752	35.246	1.00 39.59	A
ATOM	5654	CB	PRO	A	740	9.718	28.268	35.246	1.00 52.42	A
ATOM	5655	CG	PRO	A	740	9.456	28.572	33.791	1.00 52.42	A
ATOM	5656	C	PRO	A	740	9.467	26.113	36.563	1.00 39.59	A
ATOM	5657	O	PRO	A	740	10.289	25.636	37.345	1.00 39.59	A
ATOM	5658	N	VAL	A	741	8.161	26.104	36.802	1.00 40.82	A
ATOM	5659	CA	VAL	A	741	7.628	25.524	38.025	1.00 40.82	A
ATOM	5660	CB	VAL	A	741	6.137	25.852	38.174	1.00 46.44	A
ATOM	5661	CG1	VAL	A	741	5.582	25.217	39.450	1.00 46.44	A
ATOM	5662	CG2	VAL	A	741	5.954	27.357	38.189	1.00 46.44	A
ATOM	5663	C	VAL	A	741	7.799	24.010	38.012	1.00 40.82	A

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ATOM	5664	O	VAL	A	741	8.205	23.404	39.005	1.00	40.82	A
ATOM	5665	N	HIS	A	742	7.499	23.402	36.871	1.00	39.52	A
ATOM	5666	CA	HIS	A	742	7.608	21.961	36.747	1.00	39.52	A
ATOM	5667	CB	HIS	A	742	7.277	21.522	35.326	1.00	43.70	A
ATOM	5668	CG	HIS	A	742	7.385	20.046	35.122	1.00	43.70	A
ATOM	5669	CD2	HIS	A	742	6.528	19.043	35.422	1.00	43.70	A
ATOM	5670	ND1	HIS	A	742	8.490	19.451	34.551	1.00	43.70	A
ATOM	5671	CE1	HIS	A	742	8.306	18.143	34.504	1.00	43.70	A
ATOM	5672	NE2	HIS	A	742	7.123	17.870	35.029	1.00	43.70	A
ATOM	5673	C	HIS	A	742	8.994	21.464	37.105	1.00	39.52	A
ATOM	5674	O	HIS	A	742	9.147	20.554	37.914	1.00	39.52	A
ATOM	5675	N	TYR	A	743	10.010	22.063	36.494	1.00	38.31	A
ATOM	5676	CA	TYR	A	743	11.372	21.642	36.765	1.00	38.31	A
ATOM	5677	CB	TYR	A	743	12.289	22.174	35.658	1.00	45.12	A
ATOM	5678	CG	TYR	A	743	11.981	21.462	34.362	1.00	45.12	A
ATOM	5679	CD1	TYR	A	743	12.086	20.077	34.281	1.00	45.12	A
ATOM	5680	CE1	TYR	A	743	11.700	19.390	33.141	1.00	45.12	A
ATOM	5681	CD2	TYR	A	743	11.491	22.150	33.251	1.00	45.12	A
ATOM	5682	CE2	TYR	A	743	11.100	21.467	32.088	1.00	45.12	A
ATOM	5683	CZ	TYR	A	743	11.202	20.086	32.049	1.00	45.12	A
ATOM	5684	OH	TYR	A	743	10.755	19.382	30.953	1.00	45.12	A
ATOM	5685	C	TYR	A	743	11.856	21.998	38.169	1.00	38.31	A
ATOM	5686	O	TYR	A	743	12.664	21.277	38.747	1.00	38.31	A
ATOM	5687	N	ALA	A	744	11.359	23.088	38.736	1.00	40.59	A
ATOM	5688	CA	ALA	A	744	11.755	23.427	40.100	1.00	40.59	A
ATOM	5689	CB	ALA	A	744	11.083	24.719	40.549	1.00	43.93	A
ATOM	5690	C	ALA	A	744	11.318	22.265	41.001	1.00	40.59	A
ATOM	5691	O	ALA	A	744	12.074	21.802	41.861	1.00	40.59	A
ATOM	5692	N	HIS	A	745	10.101	21.782	40.775	1.00	40.98	A
ATOM	5693	CA	HIS	A	745	9.551	20.680	41.561	1.00	40.98	A
ATOM	5694	CB	HIS	A	745	8.069	20.465	41.212	1.00	68.13	A
ATOM	5695	CG	HIS	A	745	7.363	19.508	42.125	1.00	68.13	A
ATOM	5696	CD2	HIS	A	745	6.752	19.703	43.317	1.00	68.13	A
ATOM	5697	ND1	HIS	A	745	7.256	18.159	41.857	1.00	68.13	A
ATOM	5698	CE1	HIS	A	745	6.610	17.564	42.845	1.00	68.13	A
ATOM	5699	NE2	HIS	A	745	6.294	18.479	43.744	1.00	68.13	A
ATOM	5700	C	HIS	A	745	10.341	19.398	41.344	1.00	40.98	A
ATOM	5701	O	HIS	A	745	10.589	18.654	42.292	1.00	40.98	A
ATOM	5702	N	LYS	A	746	10.733	19.131	40.100	1.00	39.29	A
ATOM	5703	CA	LYS	A	746	11.513	17.932	39.819	1.00	39.29	A
ATOM	5704	CB	LYS	A	746	11.755	17.768	38.312	1.00	54.60	A
ATOM	5705	CG	LYS	A	746	10.509	17.447	37.497	1.00	54.60	A
ATOM	5706	CD	LYS	A	746	9.941	16.071	37.833	1.00	54.60	A
ATOM	5707	CE	LYS	A	746	10.830	14.954	37.303	1.00	54.60	A
ATOM	5708	NZ	LYS	A	746	10.225	13.592	37.502	1.00	54.60	A
ATOM	5709	C	LYS	A	746	12.862	18.008	40.538	1.00	39.29	A
ATOM	5710	O	LYS	A	746	13.337	17.019	41.070	1.00	39.29	A
ATOM	5711	N	PHE	A	747	13.488	19.179	40.543	1.00	36.74	A
ATOM	5712	CA	PHE	A	747	14.777	19.305	41.199	1.00	36.74	A
ATOM	5713	CB	PHE	A	747	15.427	20.646	40.860	1.00	40.07	A
ATOM	5714	CG	PHE	A	747	16.833	20.764	41.350	1.00	40.07	A
ATOM	5715	CD1	PHE	A	747	17.781	19.787	41.016	1.00	40.07	A
ATOM	5716	CD2	PHE	A	747	17.216	21.827	42.171	1.00	40.07	A
ATOM	5717	CE1	PHE	A	747	19.078	19.860	41.495	1.00	40.07	A
ATOM	5718	CE2	PHE	A	747	18.525	21.909	42.657	1.00	40.07	A
ATOM	5719	CZ	PHE	A	747	19.455	20.924	42.322	1.00	40.07	A
ATOM	5720	C	PHE	A	747	14.632	19.145	42.724	1.00	36.74	A

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ATOM	5721	O	PHE	A	747	15.399	18.411	43.354	1.00	36.74	A
ATOM	5722	N	ALA	A	748	13.643	19.811	43.306	1.00	44.70	A
ATOM	5723	CA	ALA	A	748	13.406	19.694	44.737	1.00	44.70	A
ATOM	5724	CB	ALA	A	748	12.158	20.491	45.134	1.00	34.75	A
ATOM	5725	C	ALA	A	748	13.222	18.204	45.062	1.00	44.70	A
ATOM	5726	O	ALA	A	748	13.719	17.719	46.072	1.00	44.70	A
ATOM	5727	N	ASN	A	749	12.529	17.476	44.192	1.00	45.21	A
ATOM	5728	CA	ASN	A	749	12.324	16.045	44.410	1.00	45.21	A
ATOM	5729	CB	ASN	A	749	11.366	15.457	43.368	1.00	59.26	A
ATOM	5730	CG	ASN	A	749	9.913	15.757	43.675	1.00	59.26	A
ATOM	5731	OD1	ASN	A	749	9.553	16.036	44.821	1.00	59.26	A
ATOM	5732	ND2	ASN	A	749	9.064	15.681	42.655	1.00	59.26	A
ATOM	5733	C	ASN	A	749	13.627	15.245	44.380	1.00	45.21	A
ATOM	5734	O	ASN	A	749	13.850	14.374	45.223	1.00	45.21	A
ATOM	5735	N	ALA	A	750	14.479	15.529	43.402	1.00	49.51	A
ATOM	5736	CA	ALA	A	750	15.746	14.822	43.274	1.00	49.51	A
ATOM	5737	CB	ALA	A	750	16.437	15.231	41.979	1.00	33.70	A
ATOM	5738	C	ALA	A	750	16.658	15.085	44.482	1.00	49.51	A
ATOM	5739	O	ALA	A	750	17.362	14.185	44.950	1.00	49.51	A
ATOM	5740	N	ILE	A	751	16.648	16.315	44.980	1.00	50.38	A
ATOM	5741	CA	ILE	A	751	17.459	16.662	46.144	1.00	50.38	A
ATOM	5742	CB	ILE	A	751	17.342	18.166	46.510	1.00	52.88	A
ATOM	5743	CG2	ILE	A	751	18.258	18.485	47.690	1.00	52.88	A
ATOM	5744	CG1	ILE	A	751	17.759	19.040	45.336	1.00	52.88	A
ATOM	5745	CD1	ILE	A	751	17.551	20.509	45.594	1.00	52.88	A
ATOM	5746	C	ILE	A	751	16.957	15.843	47.341	1.00	50.38	A
ATOM	5747	O	ILE	A	751	17.752	15.317	48.123	1.00	50.38	A
ATOM	5748	N	ARG	A	752	15.635	15.745	47.475	1.00	59.72	A
ATOM	5749	CA	ARG	A	752	15.033	14.983	48.564	1.00	59.72	A
ATOM	5750	CB	ARG	A	752	13.522	15.228	48.652	1.00	91.88	A
ATOM	5751	CG	ARG	A	752	13.114	16.607	49.133	1.00	91.88	A
ATOM	5752	CD	ARG	A	752	11.888	16.535	50.036	1.00	91.88	A
ATOM	5753	NE	ARG	A	752	10.793	15.787	49.427	1.00	91.88	A
ATOM	5754	CZ	ARG	A	752	10.169	16.149	48.310	1.00	91.88	A
ATOM	5755	NH1	ARG	A	752	10.528	17.257	47.675	1.00	91.88	A
ATOM	5756	NH2	ARG	A	752	9.186	15.400	47.825	1.00	91.88	A
ATOM	5757	C	ARG	A	752	15.268	13.494	48.365	1.00	59.72	A
ATOM	5758	O	ARG	A	752	15.139	12.718	49.306	1.00	59.72	A
ATOM	5759	N	ASN	A	753	15.603	13.096	47.138	1.00	55.46	A
ATOM	5760	CA	ASN	A	753	15.845	11.688	46.848	1.00	55.46	A
ATOM	5761	CB	ASN	A	753	15.153	11.276	45.545	1.00	64.92	A
ATOM	5762	CG	ASN	A	753	13.645	11.126	45.707	1.00	64.92	A
ATOM	5763	OD1	ASN	A	753	13.170	10.514	46.668	1.00	64.92	A
ATOM	5764	ND2	ASN	A	753	12.888	11.670	44.758	1.00	64.92	A
ATOM	5765	C	ASN	A	753	17.322	11.304	46.804	1.00	55.46	A
ATOM	5766	O	ASN	A	753	17.673	10.220	46.344	1.00	55.46	A
ATOM	5767	N	GLU	A	754	18.185	12.199	47.273	1.00	51.88	A
ATOM	5768	CA	GLU	A	754	19.623	11.921	47.347	1.00	51.88	A
ATOM	5769	CB	GLU	A	754	19.856	10.502	47.891	1.00	96.52	A
ATOM	5770	CG	GLU	A	754	19.132	10.172	49.191	1.00	96.52	A
ATOM	5771	CD	GLU	A	754	19.887	10.626	50.423	1.00	96.52	A
ATOM	5772	OE1	GLU	A	754	21.018	10.141	50.641	1.00	96.52	A
ATOM	5773	OE2	GLU	A	754	19.348	11.464	51.176	1.00	96.52	A
ATOM	5774	C	GLU	A	754	20.425	12.077	46.054	1.00	51.88	A
ATOM	5775	O	GLU	A	754	21.491	11.475	45.912	1.00	51.88	A
ATOM	5776	N	TRP	A	755	19.928	12.859	45.104	1.00	47.41	A
ATOM	5777	CA	TRP	A	755	20.682	13.044	43.871	1.00	47.41	A

FIGURE 25 CON'T

ATOM	5778	CB	TRP	A	755	19.811	13.659	42.772	1.00	40.13	A
ATOM	5779	CG	TRP	A	755	19.004	12.671	41.988	1.00	40.13	A
ATOM	5780	CD2	TRP	A	755	19.229	12.278	40.630	1.00	40.13	A
ATOM	5781	CE2	TRP	A	755	18.178	11.398	40.267	1.00	40.13	A
ATOM	5782	CE3	TRP	A	755	20.214	12.588	39.681	1.00	40.13	A
ATOM	5783	CD1	TRP	A	755	17.860	12.024	42.392	1.00	40.13	A
ATOM	5784	NE1	TRP	A	755	17.357	11.260	41.359	1.00	40.13	A
ATOM	5785	CZ2	TRP	A	755	18.084	10.831	38.991	1.00	40.13	A
ATOM	5786	CZ3	TRP	A	755	20.122	12.024	38.407	1.00	40.13	A
ATOM	5787	CH2	TRP	A	755	19.061	11.154	38.076	1.00	40.13	A
ATOM	5788	C	TRP	A	755	21.858	13.968	44.130	1.00	47.41	A
ATOM	5789	O	TRP	A	755	21.746	14.930	44.891	1.00	47.41	A
ATOM	5790	N	LYS	A	756	22.989	13.680	43.502	1.00	47.96	A
ATOM	5791	CA	LYS	A	756	24.144	14.543	43.666	1.00	47.96	A
ATOM	5792	CB	LYS	A	756	25.363	13.980	42.935	1.00	56.84	A
ATOM	5793	CG	LYS	A	756	26.597	14.853	43.110	1.00	56.84	A
ATOM	5794	CD	LYS	A	756	27.900	14.128	42.787	1.00	56.84	A
ATOM	5795	CE	LYS	A	756	28.049	13.833	41.307	1.00	56.84	A
ATOM	5796	NZ	LYS	A	756	29.380	13.233	41.026	1.00	56.84	A
ATOM	5797	C	LYS	A	756	23.784	15.914	43.085	1.00	47.96	A
ATOM	5798	O	LYS	A	756	23.029	16.015	42.116	1.00	47.96	A
ATOM	5799	N	ILE	A	757	24.326	16.966	43.677	1.00	58.56	A
ATOM	5800	CA	ILE	A	757	24.059	18.316	43.214	1.00	58.56	A
ATOM	5801	CB	ILE	A	757	23.677	19.206	44.410	1.00	46.28	A
ATOM	5802	CG2	ILE	A	757	23.447	20.644	43.964	1.00	46.28	A
ATOM	5803	CG1	ILE	A	757	22.424	18.621	45.072	1.00	46.28	A
ATOM	5804	CD1	ILE	A	757	21.869	19.432	46.241	1.00	46.28	A
ATOM	5805	C	ILE	A	757	25.278	18.878	42.479	1.00	58.56	A
ATOM	5806	O	ILE	A	757	26.110	19.555	43.078	1.00	58.56	A
ATOM	5807	N	LYS	A	758	25.381	18.585	41.182	1.00	49.81	A
ATOM	5808	CA	LYS	A	758	26.502	19.063	40.368	1.00	49.81	A
ATOM	5809	CB	LYS	A	758	26.704	18.174	39.137	1.00	73.65	A
ATOM	5810	CG	LYS	A	758	27.420	16.873	39.416	1.00	73.65	A
ATOM	5811	CD	LYS	A	758	28.857	17.110	39.850	1.00	73.65	A
ATOM	5812	CE	LYS	A	758	29.724	17.530	38.678	1.00	73.65	A
ATOM	5813	NZ	LYS	A	758	29.896	16.415	37.724	1.00	73.65	A
ATOM	5814	C	LYS	A	758	26.264	20.487	39.905	1.00	49.81	A
ATOM	5815	O	LYS	A	758	25.772	20.709	38.797	1.00	49.81	A
ATOM	5816	N	GLU	A	759	26.634	21.452	40.736	1.00	45.60	A
ATOM	5817	CA	GLU	A	759	26.420	22.853	40.387	1.00	45.60	A
ATOM	5818	CB	GLU	A	759	26.965	23.754	41.492	1.00	52.93	A
ATOM	5819	CG	GLU	A	759	26.155	23.586	42.767	1.00	52.93	A
ATOM	5820	CD	GLU	A	759	26.388	24.667	43.792	1.00	52.93	A
ATOM	5821	OE1	GLU	A	759	25.624	24.695	44.782	1.00	52.93	A
ATOM	5822	OE2	GLU	A	759	27.324	25.481	43.619	1.00	52.93	A
ATOM	5823	C	GLU	A	759	26.993	23.215	39.027	1.00	45.60	A
ATOM	5824	O	GLU	A	759	26.477	24.097	38.338	1.00	45.60	A
ATOM	5825	N	GLU	A	760	28.037	22.508	38.625	1.00	50.56	A
ATOM	5826	CA	GLU	A	760	28.656	22.745	37.329	1.00	50.56	A
ATOM	5827	CB	GLU	A	760	29.829	21.788	37.154	1.00	77.81	A
ATOM	5828	CG	GLU	A	760	30.544	21.897	35.829	1.00	77.81	A
ATOM	5829	CD	GLU	A	760	31.612	20.831	35.681	1.00	77.81	A
ATOM	5830	OE1	GLU	A	760	32.504	20.760	36.554	1.00	77.81	A
ATOM	5831	OE2	GLU	A	760	31.560	20.062	34.699	1.00	77.81	A
ATOM	5832	C	GLU	A	760	27.626	22.516	36.211	1.00	50.56	A
ATOM	5833	O	GLU	A	760	27.507	23.306	35.274	1.00	50.56	A

FIGURE 25 CON'T

ATOM	5834	N	PHE	A	761	26.888	21.415	36.312	1.00	40.45	A
ATOM	5835	CA	PHE	A	761	25.872	21.089	35.314	1.00	40.45	A
ATOM	5836	CB	PHE	A	761	25.491	19.603	35.421	1.00	46.40	A
ATOM	5837	CG	PHE	A	761	26.577	18.667	34.961	1.00	46.40	A
ATOM	5838	CD1	PHE	A	761	27.811	19.165	34.527	1.00	46.40	A
ATOM	5839	CD2	PHE	A	761	26.368	17.293	34.944	1.00	46.40	A
ATOM	5840	CE1	PHE	A	761	28.813	18.308	34.082	1.00	46.40	A
ATOM	5841	CE2	PHE	A	761	27.366	16.418	34.500	1.00	46.40	A
ATOM	5842	CZ	PHE	A	761	28.596	16.931	34.066	1.00	46.40	A
ATOM	5843	C	PHE	A	761	24.641	21.972	35.490	1.00	40.45	A
ATOM	5844	O	PHE	A	761	24.097	22.485	34.521	1.00	40.45	A
ATOM	5845	N	LEU	A	762	24.233	22.168	36.737	1.00	42.78	A
ATOM	5846	CA	LEU	A	762	23.064	22.977	37.058	1.00	42.78	A
ATOM	5847	CB	LEU	A	762	22.803	22.911	38.568	1.00	39.89	A
ATOM	5848	CG	LEU	A	762	22.567	21.510	39.164	1.00	39.89	A
ATOM	5849	CD1	LEU	A	762	22.491	21.589	40.699	1.00	39.89	A
ATOM	5850	CD2	LEU	A	762	21.276	20.912	38.584	1.00	39.89	A
ATOM	5851	C	LEU	A	762	23.186	24.444	36.613	1.00	42.78	A
ATOM	5852	O	LEU	A	762	22.168	25.115	36.361	1.00	42.78	A
ATOM	5853	N	ALA	A	763	24.423	24.936	36.514	1.00	43.71	A
ATOM	5854	CA	ALA	A	763	24.679	26.319	36.116	1.00	43.71	A
ATOM	5855	CB	ALA	A	763	26.098	26.736	36.552	1.00	50.06	A
ATOM	5856	C	ALA	A	763	24.510	26.537	34.614	1.00	43.71	A
ATOM	5857	O	ALA	A	763	24.491	27.674	34.139	1.00	43.71	A
ATOM	5858	N	GLU	A	764	24.398	25.442	33.870	1.00	43.52	A
ATOM	5859	CA	GLU	A	764	24.222	25.509	32.425	1.00	43.52	A
ATOM	5860	CB	GLU	A	764	25.292	24.665	31.727	1.00	62.60	A
ATOM	5861	CG	GLU	A	764	26.693	25.246	31.815	1.00	62.60	A
ATOM	5862	CD	GLU	A	764	26.866	26.463	30.932	1.00	62.60	A
ATOM	5863	OE1	GLU	A	764	27.217	26.298	29.743	1.00	62.60	A
ATOM	5864	OE2	GLU	A	764	26.632	27.587	31.425	1.00	62.60	A
ATOM	5865	C	GLU	A	764	22.831	24.989	32.064	1.00	43.52	A
ATOM	5866	O	GLU	A	764	22.534	24.737	30.903	1.00	43.52	A
ATOM	5867	N	GLY	A	765	21.988	24.806	33.074	1.00	40.66	A
ATOM	5868	CA	GLY	A	765	20.648	24.324	32.810	1.00	40.66	A
ATOM	5869	C	GLY	A	765	20.502	22.858	32.430	1.00	40.66	A
ATOM	5870	O	GLY	A	765	19.542	22.506	31.748	1.00	40.66	A
ATOM	5871	N	PHE	A	766	21.442	22.013	32.859	1.00	37.82	A
ATOM	5872	CA	PHE	A	766	21.389	20.572	32.582	1.00	37.82	A
ATOM	5873	CB	PHE	A	766	22.663	19.857	33.076	1.00	44.51	A
ATOM	5874	CG	PHE	A	766	23.860	19.974	32.170	1.00	44.51	A
ATOM	5875	CD1	PHE	A	766	24.322	21.210	31.730	1.00	44.51	A
ATOM	5876	CD2	PHE	A	766	24.597	18.834	31.846	1.00	44.51	A
ATOM	5877	CE1	PHE	A	766	25.509	21.310	30.983	1.00	44.51	A
ATOM	5878	CE2	PHE	A	766	25.778	18.922	31.104	1.00	44.51	A
ATOM	5879	CZ	PHE	A	766	26.236	20.162	30.674	1.00	44.51	A
ATOM	5880	C	PHE	A	766	20.218	19.952	33.367	1.00	37.82	A
ATOM	5881	O	PHE	A	766	20.238	19.949	34.598	1.00	37.82	A
ATOM	5882	N	LEU	A	767	19.209	19.418	32.686	1.00	38.39	A
ATOM	5883	CA	LEU	A	767	18.103	18.782	33.412	1.00	38.39	A
ATOM	5884	CB	LEU	A	767	16.802	18.925	32.616	1.00	34.83	A
ATOM	5885	CG	LEU	A	767	16.252	20.355	32.537	1.00	34.83	A
ATOM	5886	CD1	LEU	A	767	15.172	20.439	31.471	1.00	34.83	A
ATOM	5887	CD2	LEU	A	767	15.711	20.772	33.909	1.00	34.83	A
ATOM	5888	C	LEU	A	767	18.454	17.302	33.609	1.00	38.39	A
ATOM	5889	O	LEU	A	767	17.730	16.404	33.154	1.00	38.39	A
ATOM	5890	N	TYR	A	768	19.560	17.041	34.307	1.00	32.98	A

FIGURE 25 CON'T

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ATOM   5891  CA  TYR A 768      20.016  15.655  34.494  1.00 32.98      A
ATOM   5892  CB  TYR A 768      21.479  15.628  34.948  1.00 37.63      A
ATOM   5893  CG  TYR A 768      21.718  16.219  36.318  1.00 37.63      A
ATOM   5894  CD1 TYR A 768      21.427  15.499  37.479  1.00 37.63      A
ATOM   5895  CE1 TYR A 768      21.680  16.036  38.742  1.00 37.63      A
ATOM   5896  CD2 TYR A 768      22.266  17.492  36.454  1.00 37.63      A
ATOM   5897  CE2 TYR A 768      22.527  18.034  37.705  1.00 37.63      A
ATOM   5898  CZ  TYR A 768      22.233  17.310  38.845  1.00 37.63      A
ATOM   5899  OH  TYR A 768      22.488  17.874  40.081  1.00 37.63      A
ATOM   5900  C   TYR A 768      19.206  14.799  35.440  1.00 32.98      A
ATOM   5901  O   TYR A 768      19.243  13.579  35.338  1.00 32.98      A
ATOM   5902  N   PHE A 769      18.486  15.443  36.352  1.00 42.84      A
ATOM   5903  CA  PHE A 769      17.663  14.769  37.349  1.00 42.84      A
ATOM   5904  CB  PHE A 769      17.633  15.633  38.604  1.00 31.31      A
ATOM   5905  CG  PHE A 769      17.232  17.052  38.325  1.00 31.31      A
ATOM   5906  CD1 PHE A 769      15.885  17.417  38.284  1.00 31.31      A
ATOM   5907  CD2 PHE A 769      18.194  17.997  37.962  1.00 31.31      A
ATOM   5908  CE1 PHE A 769      15.505  18.686  37.881  1.00 31.31      A
ATOM   5909  CE2 PHE A 769      17.819  19.269  37.556  1.00 31.31      A
ATOM   5910  CZ  PHE A 769      16.471  19.616  37.513  1.00 31.31      A
ATOM   5911  C   PHE A 769      16.224  14.553  36.851  1.00 42.84      A
ATOM   5912  O   PHE A 769      15.406  13.941  37.540  1.00 42.84      A
ATOM   5913  N   VAL A 770      15.923  15.068  35.664  1.00 74.51      A
ATOM   5914  CA  VAL A 770      14.588  14.955  35.092  1.00 74.51      A
ATOM   5915  CB  VAL A 770      14.200  16.229  34.315  1.00 61.33      A

ATOM   5916  CG1 VAL A 770      12.799  16.097  33.781  1.00 61.33      A
ATOM   5917  CG2 VAL A 770      14.301  17.436  35.202  1.00 61.33      A
ATOM   5918  C   VAL A 770      14.477  13.785  34.132  1.00 74.51      A
ATOM   5919  O   VAL A 770      14.621  14.045  32.917  1.00 74.51      A
ATOM   5920  OXT VAL A 770      14.260  12.640  34.588  1.00 61.33      A
TER
HETATM 5921  OH2 TIP     1      18.370  21.810  29.334  1.00 44.97      S
HETATM 5922  OH2 TIP     2      21.899   9.099  35.356  1.00 40.25      S
HETATM 5923  OH2 TIP     3      17.715  23.135  26.861  1.00 45.74      S
HETATM 5924  OH2 TIP     4      -2.476  34.389  46.433  1.00 57.89      S
HETATM 5925  OH2 TIP     5     -14.987   6.046  36.915  1.00 53.30      S
HETATM 5926  OH2 TIP     6     -12.088  26.903  41.491  1.00 46.69      S
HETATM 5927  OH2 TIP     7     -13.937  25.878  43.376  1.00 45.40      S
HETATM 5928  OH2 TIP     8     -11.412  13.515  38.333  1.00 43.19      S
HETATM 5929  OH2 TIP     9      -0.863  24.163  41.344  1.00 53.53      S
HETATM 5930  OH2 TIP    10      -5.288   1.461  64.019  1.00 48.92      S
HETATM 5931  OH2 TIP    11       2.392  30.592  41.077  1.00 38.99      S
HETATM 5932  OH2 TIP    12      -0.342   0.215  47.316  1.00 46.86      S
HETATM 5933  OH2 TIP    13      -9.647  15.151  37.001  1.00 45.57      S
HETATM 5934  OH2 TIP    14     -10.301  15.778  34.084  1.00 43.77      S
HETATM 5935  OH2 TIP    15      20.555  11.259  34.330  1.00 45.20      S
HETATM 5936  OH2 TIP    16      28.742  20.816  42.795  1.00 44.99      S
HETATM 5937  OH2 TIP    17     -13.195  30.515  39.458  1.00 52.48      S
HETATM 5938  OH2 TIP    18     -11.704  20.891  31.112  1.00 42.42      S
HETATM 5939  OH2 TIP    19      -3.276   9.798  47.460  1.00 49.11      S
HETATM 5940  OH2 TIP    20      -6.804   0.216  75.536  1.00 47.88      S
HETATM 5941  OH2 TIP    21     -18.325  20.403  49.558  1.00 50.84      S
HETATM 5942  OH2 TIP    22     -16.649  26.665  47.872  1.00 47.40      S
HETATM 5943  OH2 TIP    23     -16.485  13.068  25.192  1.00 47.13      S
HETATM 5944  OH2 TIP    24     -18.046   8.967  49.052  1.00 49.94      S
HETATM 5945  OH2 TIP    25       9.520  -9.191  28.429  1.00 58.22      S
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FIGURE 25 CON'T

HETATM 5946	OH2 TIP	26	16.540	25.632	27.261	1.00 47.57	S
HETATM 5947	OH2 TIP	27	3.118	37.550	32.058	1.00 54.40	S
HETATM 5948	OH2 TIP	28	10.045	-3.931	55.270	1.00 51.11	S
HETATM 5949	OH2 TIP	29	15.202	8.781	31.435	1.00 49.91	S
HETATM 5950	OH2 TIP	30	-26.959	25.672	35.586	1.00 48.67	S
HETATM 5951	OH2 TIP	31	10.791	-9.014	26.464	1.00 59.29	S
HETATM 5952	OH2 TIP	32	-2.669	23.392	42.935	1.00 57.01	S
HETATM 5953	OH2 TIP	33	-19.309	21.014	25.827	1.00 48.36	S
HETATM 5954	OH2 TIP	34	-9.112	11.965	44.438	1.00 56.44	S
HETATM 5955	OH2 TIP	35	-26.009	29.088	33.535	1.00 53.75	S
HETATM 5956	OH2 TIP	36	-5.553	4.212	66.054	1.00 69.21	S
HETATM 5957	OH2 TIP	37	11.338	20.488	23.113	1.00 57.25	S
HETATM 5958	OH2 TIP	38	-9.515	16.282	40.382	1.00 53.65	S
HETATM 5959	OH2 TIP	39	2.189	8.728	53.259	1.00 51.62	S
HETATM 5960	OH2 TIP	40	29.893	20.655	40.220	1.00 61.64	S
HETATM 5961	OH2 TIP	41	-8.168	36.508	40.351	1.00 56.55	S
HETATM 5962	OH2 TIP	42	-16.396	37.700	39.050	1.00 57.28	S
HETATM 5963	OH2 TIP	43	-17.803	38.142	41.395	1.00 62.91	S
HETATM 5964	OH2 TIP	44	6.251	7.179	47.328	1.00 50.89	S
HETATM 5965	OH2 TIP	45	-7.728	22.337	20.181	1.00 51.49	S
HETATM 5966	OH2 TIP	46	6.036	24.040	46.517	1.00 57.58	S
HETATM 5967	OH2 TIP	47	-10.838	11.111	57.417	1.00 72.00	S
HETATM 5968	OH2 TIP	48	9.902	4.698	27.131	1.00 54.85	S
HETATM 5969	OH2 TIP	49	24.470	32.001	48.942	1.00 64.93	S
HETATM 5970	OH2 TIP	50	21.439	27.832	48.102	1.00 55.84	S
HETATM 5971	OH2 TIP	51	-23.212	4.269	47.464	1.00 52.89	S
HETATM 5972	OH2 TIP	52	8.541	4.628	44.863	1.00 68.12	S
HETATM 5973	OH2 TIP	53	-16.370	13.072	47.759	1.00 51.09	S
HETATM 5974	OH2 TIP	54	9.141	18.845	46.330	1.00 55.16	S
HETATM 5975	OH2 TIP	55	-21.814	2.461	46.114	1.00 61.78	S
HETATM 5976	OH2 TIP	56	-28.157	10.364	48.240	1.00 53.11	S
HETATM 5977	OH2 TIP	57	-27.342	32.420	42.439	1.00 51.52	S
HETATM 5978	OH2 TIP	58	-15.983	27.483	57.654	1.00 55.12	S
HETATM 5979	OH2 TIP	59	-16.252	16.477	36.469	1.00 22.88	S
HETATM 5980	OH2 TIP	60	16.220	10.260	4.698	1.00 70.64	S
HETATM 5981	OH2 TIP	61	9.900	7.126	48.174	1.00 69.93	S
HETATM 5982	OH2 TIP	62	-2.545	14.634	63.859	1.00 66.97	S
HETATM 5983	OH2 TIP	63	-25.196	4.635	45.535	1.00 51.71	S
HETATM 5984	OH2 TIP	64	-18.872	-1.352	47.305	1.00 70.97	S
HETATM 5985	OH2 TIP	65	2.709	-12.794	61.990	1.00 71.93	S
HETATM 5986	OH2 TIP	66	-11.260	-6.365	37.836	1.00 73.76	S
HETATM 5987	OH2 TIP	67	-15.786	37.673	36.314	1.00 74.43	S
HETATM 5988	OH2 TIP	68	17.880	22.397	16.014	1.00 54.49	S
HETATM 5989	OH2 TIP	69	-21.502	15.816	52.789	1.00 56.42	S
HETATM 5990	OH2 TIP	70	5.325	-0.467	16.696	1.00 60.24	S
HETATM 5991	OH2 TIP	71	11.117	22.339	24.819	1.00 61.70	S
HETATM 5992	OH2 TIP	72	23.110	11.363	42.088	1.00 46.89	S
HETATM 5993	OH2 TIP	73	21.863	-9.662	36.508	1.00 47.82	S
HETATM 5994	OH2 TIP	74	20.547	46.701	40.738	1.00 72.58	S
HETATM 5995	OH2 TIP	75	33.405	9.009	38.372	1.00 64.06	S
HETATM 5996	OH2 TIP	76	-7.459	19.056	39.490	1.00 53.56	S
HETATM 5997	OH2 TIP	77	-16.279	32.467	44.564	1.00 54.71	S
HETATM 5998	OH2 TIP	78	20.859	37.282	41.728	1.00 53.34	S
HETATM 5999	OH2 TIP	79	-9.099	5.768	64.065	1.00 53.69	S
HETATM 6000	OH2 TIP	80	17.074	48.531	37.844	1.00 57.71	S
HETATM 6001	OH2 TIP	81	-20.591	1.700	36.204	1.00 54.39	S
HETATM 6002	OH2 TIP	82	28.187	29.184	34.781	1.00 68.56	S

FIGURE 25 CON'T

HETATM	6003	OH2	TIP	83	17.032	36.198	26.598	1.00	67.39	S
HETATM	6004	OH2	TIP	84	22.262	8.106	13.250	1.00	55.06	S
HETATM	6005	OH2	TIP	85	21.630	15.662	15.725	1.00	70.89	S
HETATM	6006	OH2	TIP	86	-14.521	1.762	54.240	1.00	56.21	S
HETATM	6007	OH2	TIP	87	-5.498	-7.282	59.486	1.00	64.11	S
HETATM	6008	OH2	TIP	88	-14.952	27.909	45.106	1.00	55.41	S
HETATM	6009	OH2	TIP	89	-9.574	11.072	36.645	1.00	60.66	S
HETATM	6010	OH2	TIP	90	-19.934	26.786	19.690	1.00	61.56	S
HETATM	6011	OH2	TIP	91	-19.722	25.179	57.795	1.00	61.53	S
HETATM	6012	OH2	TIP	92	-5.179	4.991	79.116	1.00	59.85	S
HETATM	6013	OH2	TIP	93	23.200	29.231	31.436	1.00	56.39	S
HETATM	6014	OH2	TIP	94	14.477	10.996	37.967	1.00	62.57	S
HETATM	6015	OH2	TIP	95	5.075	38.959	28.482	1.00	60.07	S
HETATM	6016	OH2	TIP	96	3.783	42.153	55.054	1.00	83.33	S
HETATM	6017	OH2	TIP	97	4.878	29.768	52.759	1.00	52.19	S
HETATM	6018	OH2	TIP	98	-28.304	35.106	42.428	1.00	68.52	S
HETATM	6019	OH2	TIP	99	-6.647	-10.395	70.918	1.00	54.01	S
HETATM	6020	OH2	TIP	100	-21.038	41.643	47.045	1.00	67.28	S
HETATM	6021	OH2	TIP	101	34.025	6.004	38.783	1.00	54.10	S
HETATM	6022	OH2	TIP	102	36.250	4.424	29.906	1.00	61.46	S
HETATM	6023	OH2	TIP	103	-19.532	-2.215	42.785	1.00	68.84	S
HETATM	6024	OH2	TIP	104	-28.578	38.820	54.834	1.00	61.91	S
HETATM	6025	OH2	TIP	105	-31.547	35.211	67.941	1.00	72.99	S
HETATM	6026	OH2	TIP	106	25.271	22.710	46.374	1.00	68.08	S
HETATM	6027	OH2	TIP	107	-25.496	28.500	31.122	1.00	51.94	S
HETATM	6028	OH2	TIP	108	30.641	-4.118	25.389	1.00	61.56	S
HETATM	6029	OH2	TIP	109	-10.470	12.483	33.234	1.00	29.98	S
HETATM	6030	OH2	TIP	110	-1.801	12.520	50.029	1.00	74.36	S
HETATM	6031	OH2	TIP	111	6.173	25.074	43.601	1.00	49.94	S
HETATM	6032	OH2	TIP	112	20.958	-10.184	22.202	1.00	80.32	S
HETATM	6033	OH2	TIP	113	22.035	25.421	55.991	1.00	64.77	S
HETATM	6034	OH2	TIP	114	-30.415	16.042	33.842	1.00	57.83	S
HETATM	6035	OH2	TIP	115	5.151	24.111	49.267	1.00	58.42	S
HETATM	6036	OH2	TIP	116	-12.603	7.930	52.673	1.00	59.27	S
HETATM	6037	OH2	TIP	117	27.059	-10.195	35.988	1.00	57.86	S
HETATM	6038	OH2	TIP	118	-3.826	-5.899	43.779	1.00	51.76	S
HETATM	6039	OH2	TIP	119	-4.725	20.658	29.307	1.00	62.77	S
HETATM	6040	OH2	TIP	120	-18.107	11.820	49.900	1.00	68.29	S
HETATM	6041	OH2	TIP	121	17.151	11.758	34.731	1.00	55.47	S
HETATM	6042	OH2	TIP	122	8.014	33.927	55.929	1.00	71.42	S
HETATM	6043	OH2	TIP	123	-3.700	-4.366	41.096	1.00	77.33	S
HETATM	6044	OH2	TIP	124	0.364	19.226	44.509	1.00	61.07	S
HETATM	6045	OH2	TIP	125	-24.577	17.454	58.370	1.00	86.24	S
HETATM	6046	OH2	TIP	126	22.736	-8.506	25.854	1.00	56.67	S
HETATM	6047	OH2	TIP	127	7.925	-9.335	64.313	1.00	77.83	S
HETATM	6048	OH2	TIP	128	0.340	27.055	48.265	1.00	63.16	S
HETATM	6049	OH2	TIP	129	-3.152	41.692	27.224	1.00	52.94	S
HETATM	6050	OH2	TIP	130	-31.945	32.910	40.837	1.00	57.78	S
HETATM	6051	OH2	TIP	131	16.495	37.467	29.440	1.00	60.34	S
HETATM	6052	OH2	TIP	132	-9.277	38.782	34.372	1.00	67.29	S
HETATM	6053	OH2	TIP	133	-1.692	32.663	53.014	1.00	71.19	S
HETATM	6054	OH2	TIP	134	-15.239	34.373	42.234	1.00	64.11	S
HETATM	6055	OH2	TIP	135	9.945	15.897	33.414	1.00	70.18	S
HETATM	6056	OH2	TIP	136	26.089	32.855	33.020	1.00	73.49	S
HETATM	6057	OH2	TIP	137	-1.929	26.327	46.767	1.00	64.01	S
HETATM	6058	OH2	TIP	138	13.583	11.648	31.478	1.00	60.15	S
HETATM	6059	OH2	TIP	139	-7.307	-6.874	73.320	1.00	63.01	S

FIGURE 25 CON'T

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HETATM 6060  OH2 TIP   140       9.685  -0.304  44.722  1.00 73.65      S
HETATM 6061  OH2 TIP   141      -9.735  19.821  43.417  1.00 71.29      S
HETATM 6062  OH2 TIP   142      13.163  34.923  21.459  1.00 68.38      S
HETATM 6063  OH2 TIP   143      26.022  30.090  31.402  1.00 68.11      S
HETATM 6064  OH2 TIP   144     -27.679   1.275  40.061  1.00 63.18      S
HETATM 6065  OH2 TIP   145      14.352  31.000  21.838  1.00 55.20      S
HETATM 6066  OH2 TIP   146       2.168  46.394  49.629  1.00 60.35      S
HETATM 6067  OH2 TIP   147      17.351   9.774  33.057  1.00 69.92      S
HETATM 6068  OH2 TIP   148      22.741  27.792  29.446  1.00 67.41      S
HETATM 6069  OH2 TIP   149      25.467  17.052  46.437  1.00 51.85      S
HETATM 6070  OH2 TIP   150      -8.133  12.899  35.603  1.00 51.72      S
HETATM 6071  OH2 TIP   151      39.496  12.986  32.142  1.00 62.69      S
HETATM 6072  OH2 TIP   152     -27.004  20.006  31.382  1.00 55.79      S
HETATM 6073  OH2 TIP   153      11.578  47.500  43.124  1.00 55.79      S
HETATM 6074  OH2 TIP   154     -20.336  32.675  28.580  1.00 55.17      S
HETATM 6075  OH2 TIP   155      13.097 -10.641  36.782  1.00 68.86      S
HETATM 6076  OH2 TIP   156       5.383   2.741  40.628  1.00 76.91      S
HETATM 6077  OH2 TIP   157       0.299  -0.391  44.871  1.00 75.15      S
HETATM 6078  OH2 TIP   158      18.732  30.891  19.910  1.00 57.45      S
HETATM 6079  OH2 TIP   159      11.519  16.830  31.002  1.00 66.16      S
HETATM 6080  OH2 TIP   160       5.770  13.582  62.799  1.00 90.10      S
HETATM 6081  OH2 TIP   161     -19.600  23.788  55.119  1.00 63.82      S
HETATM 6082  OH2 TIP   162      12.071  48.060  40.615  1.00 68.92      S
HETATM 6083  OH2 TIP   163      28.289  31.551  33.446  1.00 58.67      S
HETATM 6084  OH2 TIP   164     -18.857  40.608  48.467  1.00 70.70      S
HETATM 6085  OH2 TIP   165      -2.972   6.632  69.087  1.00 71.62      S
HETATM 6086  OH2 TIP   166       5.019  21.239  11.590  1.00 74.98      S
HETATM 6087  OH2 TIP   167      -4.242 -12.300  64.349  1.00 74.41      S
HETATM 6088  OH2 TIP   168       6.092   5.418  11.062  1.00 58.26      S
HETATM 6089  OH2 TIP   169      -9.930 -16.166  70.042  1.00 77.12      S
HETATM 6090  OH2 TIP   170      27.665  32.448  46.853  1.00 86.11      S
HETATM 6091  OH2 TIP   171     -26.013  31.633  34.322  1.00 63.66      S
HETATM 6092  OH2 TIP   172       8.244   2.428  72.981  1.00 72.20      S
HETATM 6093  OH2 TIP   173     -19.875  32.340  20.985  1.00 65.25      S
HETATM 6094  OH2 TIP   174      11.462  -2.190   5.568  1.00 75.60      S
HETATM 6095  OH2 TIP   175     -24.510   4.225  34.154  1.00 65.70      S
HETATM 6096  OH2 TIP   176       9.210  19.021  23.310  1.00 53.96      S
HETATM 6097  OH2 TIP   177     -18.628  25.940  53.835  1.00 55.14      S
HETATM 6098  OH2 TIP   178       1.594  35.321  17.143  1.00 66.35      S
HETATM 6099  OH2 TIP   179     -35.932  32.773  43.500  1.00 65.83      S
HETATM 6100  OH2 TIP   180       6.610   0.656  77.404  1.00 68.12      S
HETATM 6101  OH2 TIP   181      38.280   4.139  33.513  1.00 76.88      S
HETATM 6102  OH2 TIP   182      23.197  32.109  31.628  1.00 65.86      S
HETATM 6103  OH2 TIP   183       0.495  11.928  51.178  1.00 76.94      S
HETATM 6104  OH2 TIP   184      -9.293  15.487  45.977  1.00 77.80      S
HETATM 6105  OH2 TIP   185      -5.859  38.883  39.260  1.00 53.48      S
HETATM 6106  OH2 TIP   186     -33.933  18.831  40.589  1.00 72.18      S
HETATM 6107  OH2 TIP   187       5.875  12.627  58.910  1.00 79.98      S
HETATM 6108  OH2 TIP   188       2.542  10.779  55.129  1.00 69.62      S
HETATM 6109  OH2 TIP   189       6.354  22.715  29.312  1.00 83.68      S
HETATM 6110  OH2 TIP   190      10.534  12.785  55.689  1.00 68.13      S
HETATM 6111  OH2 TIP   191     -19.033   3.122  60.501  1.00 71.79      S
HETATM 6112  OH2 TIP   192      15.573   5.668  55.157  1.00 82.05      S
END
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FIGURE 25 CON'T